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Calculation of $\langle p|\overline{u}u - \overline{d}d|p\rangle$ from QCD sum rule and the neutron-proton mass difference

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Abstract

The proton matrix element of the isovector-scalar density, $\langle p|\overline{u}u-\overline{d}d|p\rangle/2M_p$, is calculated by evaluating the nucleon current correlation function in an external isovector-scalar field using the QCD sum-rule method. In addition to the usual chiral and gluon condensates of the QCD vacuum, the response of the chiral condensates to the external isovector field enters the calculation. The latter is determined by two independent methods. One relates it to the difference between the up and down quark chiral condensates and the other uses the chiral perturbation theory. To first order in the quark mass difference $\delta m = m_d - m_u$, the non-electromagnetic part of the neutron-proton mass difference is given by the product $\delta m\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$; the resulting value is in reasonable agreement with the experimental value.

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I. INTRODUCTION

Understanding the properties of the nucleon is of obvious importance in hadron physics. A variety of nucleon matrix elements of bilinear quark operators have been evaluated in the past using various approaches. The QCD sum-rule method originally proposed by Shifman, Vainstein, and Zakharov [1] and its extension by Ioffe and Smilga [2] for external field problems, provide a tractable framework for the study of these nucleon matrix elements. These include the matrix element of electromagnetic current to determine the magnetic moments [2–4], the matrix element of the axial vector current to find the renormalization of nucleon axial coupling constant [5,6], the matrix element of the quark part of the energy momentum tensor, which gives the momentum fraction carried by the up and down quarks in deep inelastic scattering [7,8], and the matrix element of isoscalar-scalar current for evaluating the nucleon Sigma term [9]. In the present work, we calculate the matrix element of the isovector-scalar density, $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$, following the same external field approach.

The appearance of the external field leads to specific new features in QCD sum rules which distinguish them from those in the absence of the external field. Thus the phenomenological representation of the correlation function written in terms of physical intermediate states contains a double pole at the nucleon mass whose residue contains the matrix element of interest. In addition there are single pole terms which arise from the transition matrix element between the ground state nucleon and excited states. These later contributions are not exponentially damped after Borel transformation relative to the double pole term and should be retained in a consistent analysis of the sum rules. In the theoretical side of the sum rules expressed in terms of an operator product expansion (OPE) the external field contributes in two different ways–by directly coupling to the quark fields in the nucleon current and by polarizing the QCD vacuum.

Since for our problem the external field is a Lorentz scalar, non-scalar correlators cannot be induced in the QCD vacuum. However the external field does modify the quark and gluon condensates already present in the QCD vacuum. It turns out that for the problem under study the most important one is the response of the up and down quark chiral condensates to the external field which can be described by a susceptibility χ. This can be determined by writing a spectral representation, which can be evaluated for example by using chiral perturbation theory. Alternatively, since in the real world up and down quark masses are different, $\delta m = m_d - m_u$ itself can be regarded as an external isovector scalar field and χ can be related to the isospin breaking in quark condensates $\gamma \equiv (\langle 0|\overline{d}d - \overline{u}u|0\rangle)/\langle 0|\overline{u}u|0\rangle$ and is given to first order in δm by $\chi = -\gamma/\delta m$. At the current level of accuracy where these two determinations can be done, they are mutually consistent.

In Sec. II we derive the sum rules for the nucleon current correlation function in an external isovector-scalar field and describe the analysis of these sum rules, which leads us to determine $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$. We also study its dependence on the χ value.

In Sec. III we show that an evaluation of the matrix element $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$ enables us to compute the non-electromagnetic part of the neutron-proton mass difference. Since the 1970 's it has been recognized that the empirical mass difference arises from two sources. One is purely electromagnetic and yields a contribution of $-0.76 \pm 0.30\,\mathrm{MeV}$ [10] to the neutron-proton mass difference. The second source is the difference between up and down quark masses, which is of the order of the quark masses themselves. This difference leads to larger contribution which overrides the electromagnetic contribution making neutron heavier than proton. To first order in δm this later contribution is given by the product of δm and $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$.

Recently several authors [11–14] have applied the QCD sum rules for the nucleon mass to extract the neutron-proton mass difference by including the up and down quark masses in the mass sum rules for proton and neutron and the isospin breaking in the condensates. The relation of these works to ours is described in Sec. IV, where we also briefly comment on the Nolen-Schiffer anomaly.

II. SUM-RULE CALCULATION

The procedure that we use for calculating the matrix element $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$ follows the same pattern as used in Refs. [2–9]. We first couple the quarks to an external isovector-scalar field $S_V(x)$ which is described by adding a term $\Delta\mathcal{L}$ to the usual QCD Lagrangian

$$\Delta\mathcal{L} \equiv -S_V(x)[\overline{u}(x)u(x) - \overline{d}(x)d(x)] \ . \tag{2.1}$$

We can take $S_V(x)$ to be a constant S_V since we are only interested in the zero momentum transfer matrix element. The correlation functions of the nucleon current in QCD vacuum in the presence of S_V will be computed. The term linear in S_V gives the matrix element of interest.

A. QCD sum rules for $\langle p|\overline{u}u - \overline{d}d|p\rangle$

Consider the correlation function of the proton interpolating field in the presence of a *constant* external isovector-scalar field $S_{\rm V}$ which can be taken to be arbitrarily small

$$\Pi(S_{\rm V}, q) \equiv i \int d^4x e^{iq\cdot x} \langle 0|\mathrm{T}[\eta_p(x)\overline{\eta}_p(0)]\rangle_{S_{\rm V}} \ , \tag{2.2}$$

where η_p is the proton interpolating field introduced in Ref. [15]

$$\eta_p(x) = \epsilon_{abc}\left[u_a^T(x)C\gamma_\mu u_b(x)\right]\gamma_5\gamma^\mu d_c(x) \ , \tag{2.3}$$

where $u_a(x)$ and $d_c(x)$ stand for the up and down quark fields, a, b and c are the color indices, and $C = -C^T$ is the charge conjugation matrix. Since S_V is a scalar, Lorentz covariance and parity allow one to decompose $\Pi(S_{\rm V}, q)$ into two distinct structures

$$\Pi(S_{\rm V}, q) \equiv \Pi^1(S_{\rm V}, q^2) + \Pi^q(S_{\rm V}, q^2)\not{q} \ . \tag{2.4}$$

To the first order in the external field $S_{\rm V}$, the two invariant functions can be written as

$$\Pi^i(S_{\rm V}, q^2) = \Pi^i_0(q^2) + S_{\rm V}\Pi^i_1(q^2) \tag{2.5}$$

for $\{i = 1, q\}$, where Π^i_0 are the invariant functions in the absence of the external field which give rise to the mass sum rules discussed extensively in Refs. [15–18]. We are concerned here with the linear response to the external field given by $\Pi^i_1(q^2)$.

To derive a QCD sum rule, one first carries out an OPE, which will express $\Pi_1^i(q^2)$ in terms of various vacuum correlators, and then matches it to an expansion in terms of physical intermediate states. Now the external field contributes to $\Pi(S_{\rm V}, q)$ in two ways: it couples directly to the quark fields in the propagating nucleon current and it also polarizes the QCD vacuum. The chiral condensates of up and down quarks change as follows

$$\langle \overline{u}u\rangle_{S_{\rm V}} = \langle \overline{u}u\rangle_0 - \chi S_{\rm V}\langle \overline{u}u\rangle_0, \tag{2.6}$$

$$\langle \overline{d}d\rangle_{S_{\rm V}} = \langle \overline{d}d\rangle_0 + \chi S_{\rm V}\langle \overline{d}d\rangle_0, \tag{2.7}$$

where $\langle \hat{O}\rangle_0 \equiv \langle 0|\hat{O}|0\rangle$. Using Eq. (2.1) it is easy to see that χ is related to the correlation function

$$\chi\langle \overline{u}u\rangle_0 \equiv \frac{i}{2}\int d^4x \langle {\rm T}\{\overline{u}(x)u(x) - \overline{d}(x)d(x), \overline{u}(0)u(0) - \overline{d}(0)d(0)\}\rangle_0\ . \tag{2.8}$$

Similarly the mixed quark-gluon condensates change as follows

$$\langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_{S_{\rm V}} = \langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_0 - \chi_m S_{\rm V}\langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_0, \tag{2.9}$$

$$\langle g_s\overline{d}\sigma\cdot\mathcal{G}d\rangle_{S_{\rm V}} = \langle g_s\overline{d}\sigma\cdot\mathcal{G}d\rangle_0 + \chi_m S_{\rm V}\langle g_s\overline{d}\sigma\cdot\mathcal{G}d\rangle_0, \tag{2.10}$$

where $\sigma\cdot\mathcal{G} \equiv \sigma_{\mu\nu}\mathcal{G}^{\mu\nu}$ with $\mathcal{G}^{\mu\nu}$ the gluon field tensor and $\chi_{\rm m}$, the susceptibility corresponding to the quark-gluon mixed condensate, can also be expressed in terms of a spectral representation.

Since isospin is a good symmetry for hadron matrix elements we have assumed that the response of the up and down quarks is the same, apart from sign, and that we can disregard the vchange in the gluon condensate $\langle(\alpha_s/\pi)G^2\rangle$ due to the external isovector field.

To calculate the Wilson coefficients of the OPE, we need the coordinate-space quark propagators in the presence of the external field and the vacuum condensates. To first order in the external field $S_{\rm V}$, the propagators in the fixed-point gauge [19–21] take the form

$$\begin{aligned}\langle {\rm T}[u_i^a(x)\overline{u}_j^b(0)]\rangle_{S_{\rm V}} = {} & \frac{i}{2\pi^2}\delta^{ab}\frac{1}{x^4}\,[\hat{x}]_{ij} - \delta^{ab}\frac{S_{\rm V}}{4\pi^2}\frac{\delta_{ij}}{x^2} - \frac{1}{12}\delta^{ab}\langle\overline{u}u\rangle_0\delta_{ij} \\ & + \frac{1}{12}\delta^{ab}\chi S_{\rm V}\langle\overline{u}u\rangle_0\delta_{ij} + \delta^{ab}\frac{iS_{\rm V}}{48}\langle\overline{u}u\rangle_0\,[\not{x}] \\ & - \delta^{ab}\frac{x^2}{192}\langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_0\delta_{ij} - \delta^{ab}\chi_{\rm m}S_{\rm V}\frac{x^2}{192}\langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_0\delta_{ij} \\ & + \delta^{ab}\frac{iS_{\rm V}x^2}{9\cdot 128}\langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_0\,[\not{x}]_{ij} \\ & - \frac{ig_s}{32\pi^2}\left(G_{\mu\nu}(0)\right)^{ab}\frac{1}{x^2}[\not{x}\sigma^{\mu\nu} + \sigma^{\mu\nu}\not{x}]_{ij} + \cdots\ ,\end{aligned} \tag{2.11}$$

$$
\begin{aligned}
\langle \mathrm{T}[d_i^a(x)\overline{d}_j^b(0)]\rangle_{S_{\rm V}} = {} & \frac{i}{2\pi^2}\delta^{ab}\frac{1}{x^4}\,[\hat{x}]_{ij} + \delta^{ab}\frac{S_{\rm V}}{4\pi^2}\frac{\delta_{ij}}{x^2} - \frac{1}{12}\delta^{ab}\langle\overline{d}d\rangle_0\delta_{ij} \\
& -\frac{1}{12}\delta^{ab}\chi S_{\rm V}\langle\overline{d}d\rangle_0\delta_{ij} - \delta^{ab}\frac{iS_{\rm V}}{48}\langle\overline{d}d\rangle_0\,[\not{x}] \\
& -\delta^{ab}\frac{x^2}{192}\langle g_s\overline{d}\sigma\cdot\mathcal{G}d\rangle_0\delta_{ij} + \delta^{ab}\chi_{\rm m}S_{\rm V}\frac{x^2}{192}\langle g_s\overline{d}\sigma\cdot\mathcal{G}d\rangle_0\delta_{ij} \\
& -\delta^{ab}\frac{iS_{\rm V}x^2}{9\cdot 128}\langle g_s\overline{d}\sigma\cdot\mathcal{G}d\rangle_0\,[\not{x}]_{ij} \\
& -\frac{ig_s}{32\pi^2}\left(G_{\mu\nu}(0)\right)^{ab}\frac{1}{x^2}[\not{x}\sigma^{\mu\nu} + \sigma^{\mu\nu}\not{x}]_{ij} + \cdots\ . \qquad (2.12)
\end{aligned}
$$

Here we are interested in terms linear in $S_{\rm V}$. We can then disregard the current quark masses because they make negligible contributions.

The correlation function $\Pi(S_{\rm V},q)$ can be computed using the Eqs. (2.11) and (2.12) above. We have computed the contributions corresponding to the diagrams listed in Fig. 1. The results of our calculations for the invariant functions Π_1^q and Π_1^1 are

$$
\begin{aligned}
\Pi_1^q(q^2) = {} & \frac{1}{4\pi^2}\langle\overline{d}d\rangle_0\ln(-q^2) + \frac{4}{3}\chi\langle\overline{u}u\rangle_0^2\frac{1}{q^2} - \frac{1}{24\pi^2}\left(2\langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_0 - \langle g_s\overline{d}\sigma\cdot\mathcal{G}d\rangle_0\right)\frac{1}{q^2} \\
& +\frac{\chi}{6}\langle\overline{u}u\rangle_0\langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_0\frac{1}{q^4} + \frac{\chi_{\rm m}}{6}\langle\overline{u}u\rangle_0\langle g_s\overline{u}\sigma\cdot\mathcal{G}u\rangle_0\frac{1}{q^4}\ , \qquad (2.13)
\end{aligned}
$$

$$
\Pi_1^1(q^2) = \frac{1}{32\pi^4}(q^2)^2\ln(-q^2) + \frac{\chi}{4\pi^2}\langle\overline{d}d\rangle_0 q^2\ln(-q^2) - \frac{2}{3}\left(3\langle\overline{u}u\rangle_0\langle\overline{d}d\rangle_0 - 2\langle\overline{u}u\rangle_0^2\right)\frac{1}{q^2}\ . \qquad (2.14)
$$

We now turn to the phenomenological side of the sum rules, which is obtained by expanding $\Pi(S_{\rm V},q)$ in terms of physical hadronic intermediate states. There are three types of contributions. Firstly the matrix element of interest is contained in the term

$$
\langle 0|\eta_p|p\rangle\langle p|\overline{u}u - \overline{d}d|p\rangle\langle p|\overline{\eta}_p|0\rangle\ , \qquad (2.15)
$$

where the current $\overline{\eta}_p$ creates a proton that interacts with the external field $S_{\rm V}$ and is then annihilated by the current η_p. Defining

$$
\langle 0|\eta_p|p\rangle = \lambda_p v\ , \qquad (2.16)
$$

where λ_p denotes the coupling between $\overline{\eta}_p(0)|0\rangle$ and the physical proton state and v is the usual Dirac spinor ($\overline{v}v = 2M_p$), and introducing the notation

$$
H \equiv \frac{\langle p|\overline{u}u - \overline{d}d|p\rangle}{2M_p}\ , \qquad (2.17)
$$

one can write the contribution of Eq. (2.15) to $\Pi_1^i(q^2)$ as

$$
-\lambda_p^2\frac{\not{q} + M_p}{q^2 - M_p^2}\ H\ \frac{\not{q} + M_p}{q^2 - M_p^2}\ . \qquad (2.18)
$$

It is seen that the above term has a double pole at the nucleon mass.

The external field $S_{\rm V}$ can also cause transition between the proton and an excited state which can have either positive or negative parity relative to the proton. When the relative parity is positive, the contribution can be written as

$$-\lambda_p\lambda_{p^*}\frac{\not{q}+M_p}{q^2-M_p^2}\; H^*\; \frac{\not{q}-M^*}{q^2-M^{*2}}\;. \tag{2.19}$$

where now H^* is the transition matrix element between $|p\rangle$ and $|p^*\rangle$. This term has a simple pole at the proton mass as well as at the mass M^* of the excited state. It is easy to see that after a Borel transformation this contribution is not exponentially damped as compared to the double pole contribution Eq. (2.18). Therefore, one has to retain these simple pole terms in the analysis of the sum rules through the introduction of a phenomenological parameter to be determined along with the diagonal matrix element H (see Refs. [2–9]). The third type of contributions comes from transitions involving only the excited states. These are of course exponentially damped after a Borel transformation and can be approximated in the usual manner [15–18], by equating them to the perturbative contributions starting from an effective threshold.

Equating the OPE results Eqs. (2.14) and (2.13) and the physical intermediate state expansion discussed above and applying the Borel transformation [1], we obtain the following sum rules

$$\frac{M^2}{4\pi^2}\langle\overline{q}q\rangle_0 E_0 L^{-4/9}+\frac{4}{3}\chi\langle\overline{q}q\rangle_0^2 L^{4/9}-\frac{1}{24\pi^2}\langle g_s\overline{q}\sigma\cdot Gq\rangle_0 L^{-8/9}-\frac{\chi}{6M^2}\langle\overline{q}q\rangle_0\langle g_s\overline{q}\sigma\cdot Gq\rangle_0 L^{-2/27}$$
$$-\frac{\chi_m}{6M^2}\langle\overline{q}q\rangle_0\langle g_s\overline{q}\sigma\cdot Gq\rangle_0 L^{-2/27}=\left[2\lambda_p^2\frac{M_p}{M^2}H+A_q\right]e^{-M_p^2/M^2}\;, \tag{2.20}$$

$$\frac{M^6}{16\pi^4}E_2L^{-8/9}+\frac{\chi}{4\pi^2}\langle\overline{q}q\rangle_0 M^4E_1-\frac{2}{3}\langle\overline{q}q\rangle_0^2$$
$$=\left[2\lambda_p^2\frac{M_p^2}{M^2}H+A_1\right]e^{-M_p^2/M^2}\;, \tag{2.21}$$

where A_1 and A_q are the phenomenological parameters that represent the sum over the contributions from all off-diagonal transitions between the proton and the excited states. Here we have defined $E_0\equiv 1-e^{-s_0/M^2}$, $E_1\equiv 1-e^{-s_0/M^2}\left(\frac{s_0}{M^2}+1\right)$ and $E_2\equiv 1-e^{-s_0/M^2}\left(\frac{s_0}{2M^4}+\frac{s_0}{M^2}+1\right)$, which account for the sum of the contributions involving excited states only, where s_0 is an effective continuum threshold. In Eqs. (2.20) and (2.21), we have ignored the isospin breaking in the vacuum condensates. We have also taken into account the anomalous dimension of the various operators through the factor $L\equiv\ln(M^2/\Lambda_{\rm QCD}^2)/\ln(\mu^2/\Lambda_{\rm QCD}^2)$ [1,15]. We take the renormalization scale μ and the QCD scale parameter $\Lambda_{\rm QCD}$ to be 500 MeV and 150 MeV.

B. Estimate of χ

It is clear from Eq. (2.8) that χ is determined once the isovector-scalar two point function is known. The latter has been studied by Gasser and Leutwyler using chiral perturbation theory to one loop [22]. They found

$$i\int d^4x\langle 0|\mathrm{T}\{\overline{u}(x)u(x)-\overline{d}(x)d(x),\overline{u}(0)u(0)-\overline{d}(0)d(0)\}|0\rangle = 8\left(\frac{m_\pi^2}{m_u+m_d}\right)^2 h_3 \; . \qquad (2.22)$$

Since two pions cannot form an isovector-scalar, the $|\pi\pi\rangle$ intermediate state does not contribute in Eq. (2.22). The other possible pseudoscalar two particle states are $|K\overline{K}\rangle$ and $|\eta\pi\rangle$ which means that an extension to $SU(3)$ flavor symmetry is necessary. This has been done by Gasser and Leutwyler in Ref. [23]. Using Eq. (11.6) of Ref. [23], and $\langle\overline{s}s\rangle_0/\langle\overline{q}q\rangle_0=0.8$, we get $h_3\simeq -0.003$. Combining Eqs. (2.8) and (2.22), we obtain

$$\chi = -4\frac{m_\pi^2}{(m_u+m_d)f_\pi^2}h_3 \simeq 2.2\,\mathrm{GeV}^{-1} \; , \qquad (2.23)$$

where we have used $(m_u+m_d)\langle\overline{q}q\rangle_0=-m_\pi^2 f_\pi^2$, and the experimental values $m_\pi=138\,\mathrm{MeV}$, $f_\pi=93\,\mathrm{MeV}$, and a median value $\langle\overline{q}q\rangle_0=-(240\mathrm{MeV})^3$ which corresponds to $m_u+m_d=11.8\,\mathrm{MeV}$. Alternatively, χ can be determined as follows. The terms proportional to the current quark masses in the QCD Lagrangian can be written as

$$\mathcal{L}_{\mathrm{mass}} = -\hat{m}(\overline{u}u+\overline{d}d)+\frac{1}{2}\delta m(\overline{u}u-\overline{d}d)-m_s\overline{s}s-\cdots \; , \qquad (2.24)$$

where $\hat{m}\equiv\frac{1}{2}(m_u+m_d)$ and the ellipses denote the terms due to heavier quarks. Treating $\delta m(\overline{u}u-\overline{d}d)$ as a source term one obtains using Eq. (2.8)

$$\chi\langle\overline{u}u\rangle_0 = \frac{d}{d\delta m}\langle\overline{u}u-\overline{d}d\rangle_0 \; . \qquad (2.25)$$

On the other hand, one can expand $\langle\overline{u}u-\overline{d}d\rangle_0$ and $\frac{d}{d\delta m}\langle\overline{u}u-\overline{d}d\rangle_0$ into the Taylor Series in δm. Using $\langle\overline{u}u-\overline{d}d\rangle_0|_{\delta m=0}=0$, we find

$$\langle\overline{u}u-\overline{d}d\rangle_0 = \chi\delta m\langle\overline{u}u\rangle_0 + O[(\delta m)^2] \; , \qquad (2.26)$$

which implies

$$\chi\delta m = -\gamma + O[(\delta m)^2] \; . \qquad (2.27)$$

Therefore, to the lowest order in δm, the susceptibility χ is determined by the ratio of the isospin breaking parameters γ and δm. The value of γ has been estimated previously in various approaches [23–29], with results ranging from -1×10^{-2} to -3×10^{-3}. Gasser and Leutwyler [22] have determined the ratio $\delta m/(m_u+m_d)=0.28\pm0.03$. Since we have used a median value of 11.8 MeV for the sum of the up and down quark masses we adopt a median value for $\delta m=3.3\,\mathrm{MeV}$. Here we consider the γ values to be in the range -1×10^{-2} to -3×10^{-3}, which, upon using Eq. (2.27), corresponds to

$$0.9\,\mathrm{GeV}^{-1}\leq\chi\leq 3\,\mathrm{GeV}^{-1} \; . \qquad (2.28)$$

The susceptibility χ_m can also be determined using a spectral representation for Eqs. (2.9) and (2.10). However, given the uncertainty in the value of χ, we assume, in this work, $\chi_m\simeq\chi$.

C. Sum-rule analysis

Defining $a \equiv -4\pi^2\langle\overline{q}q\rangle_0$, $\tilde{\lambda}_p^2 \equiv 32\pi^4\lambda_p^2$, $m_0^2 \equiv \langle\overline{q}g_s\sigma\cdot Gq\rangle_0/\langle\overline{q}q\rangle_0$, $\tilde{A}_q = (2\pi)^4 A_q$, and $\tilde{A}_1 = (2\pi)^4 A_1$, we can rewrite the sum rules Eqs. (2.21) and (2.20) as

$$e^{M_p^2/M^2}\left[-M^4 a E_0 L^{-4/9} + \frac{4M^2}{3}\chi a^2 L^{4/9} + \frac{M^2}{6}m_0^2 a L^{-8/9} - \frac{\chi}{3}a^2 m_0^2 L^{-2/27}\right]$$
$$= \tilde{\lambda}_p^2 M_p H + \tilde{A}_q M^2 \ , \tag{2.29}$$

$$e^{M_p^2/M^2}\left[M^8 E_2 L^{-8/9} - M^6\chi a E_1 - \frac{2}{3}M^2 a^2\right]$$
$$= \tilde{\lambda}_p^2 M_p^2 H + \tilde{A}_1 M^2 \ . \tag{2.30}$$

To extract $H = \langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$, $\tilde{A}_q$ and $\tilde{A}_1$ from the above sum rules, we use the experimental value for the proton mass M_p and extract $\tilde{\lambda}_p^2$ from the proton *mass* sum rules. Using $a = 0.55\,\mathrm{GeV}^3(m_u + m_d = 11.8\,\mathrm{MeV})$ and $m_0^2 = 0.8\,\mathrm{GeV}^2$, one finds from the best fit of the proton mass sum rules that $\tilde{\lambda}_p^2 = 2.1\,\mathrm{GeV}^6$ corresponding to $s_0 = 2.3\,\mathrm{GeV}^2$ [2].We use only the first or the chiral-odd sum rule of Ioffe which is more accurate than the second or the chiral-even sum rule.

First consider the sum rule Eq. (2.29), which is obtained from $\Pi_1^q(q^2)$. For definiteness we take for χ the value $\chi = 2.2\,\mathrm{GeV}^{-1}$ given in Eq. (2.23). In Fig. 2, we plot the individual terms in the LHS of Eq. (2.29) as well as their sum, as functions of M^2 in the interval $0.8 \leq M^2 \leq 1.4\,\mathrm{GeV}^2$. It can be seen that the LHS follows a linear behavior in M^2 and we can match it with the RHS. To find the best values for the constant and the coefficient of the linear term in the RHS we follow the numerical optimization procedure used in Refs. [17,30]. We sample the sum rules in the fiducial region of M^2, where the contributions from the highest-dimensional condensates included in the sum rule remain small and the continuum contribution is controllable. Here we choose $0.8 \leq M^2 \leq 1.4\,\mathrm{GeV}^2$ as the optimization region, which is identified by Ioffe and Smilga [2] as the fiducial region for the nucleon mass sum rules. To quantify the fit of the left- and right-hand sides, we use the logarithmic measure

$$\delta(M^2) = \ln\left[\frac{\text{maximum}\{LHS, RHS\}}{\text{minimum}\{LHS, RHS\}}\right] \ , \tag{2.31}$$

which is averaged over 100 points evenly spaced within the fiducial region of M^2, where LHS and RHS denote the left- and right-hand sides of the sum rules respectively. The sum-rule predictions are obtained by minimizing δ. Using this procedure we obtain

$$H \simeq 0.54 \ , \ \tilde{A}_q \simeq 0.29\,\mathrm{GeV}^5 \ . \tag{2.32}$$

The RHS of Eq. (2.29) with these optimized values is also plotted in Fig.2. One can see that the LHS and RHS have a very good overlap.

We now turn to the other sum rule Eq. (2.30), which is obtained from Π_1^1. In Fig. 3, the individual terms in the LHS as well as their sum are shown as functions of M^2 for

$\chi = 2.2\,\mathrm{GeV}^{-1}$. The LHS is fairly linear in M^2 in the interval $0.8 \leq M^2 \leq 1.4\mathrm{GeV}^{-2}$. The RHS of Eq. (2.30), with the optimized values

$$H \simeq 0.01\ ,\ \tilde{A}_1 \simeq -1.82\,\mathrm{GeV}^6\ , \tag{2.33}$$

is also shown in Fig. 3.

It is worth noting that in the sum rule Eq. (2.29) the double pole term is more important than the single pole term, which is also qualitatively evident from the near constancy of the LHS as a function of M^2. In contrast, the single pole term in the sum rule Eq. (2.30) clearly dominates, leading us to suspect that it is not reliable to determine the double pole term in which we are interested. This is confirmed by the following.

Let us consider relaxing our tacit assumption that the continuum threshold used in our external field sum rules should be the same as the one occurring in Ioffe's mass sum rules. If s_0 is varied from $2.3\mathrm{GeV}^2$ to $2\mathrm{GeV}^2$ or $2.6\mathrm{GeV}^2$, the result for the matrix element H extracted from the sum rule Eq. (2.30) changes from 0.01 to -0.07 ($s_0 = 2\mathrm{GeV}^2$) or $+0.08$ ($s_0 = 2.6\mathrm{GeV}^2$) while the result from the sum rule Eq. (2.29) changes only from 0.54 to 0.52 or 0.56.

It is clear from the above analysis that the chiral-odd sum rule Eq. (2.29) is extremely stable, while the chiral-even sum rule Eq. (2.30) is not. So, in this paper we shall disregard the results based on the sum rule Eq. (2.30) and consider only the results from the stable sum rule Eq. (2.29).

The fact that one of the sum rules works well, while the other fails, is not peculiar to the problem under study. This pattern is seen also in a study of the isoscalar-scalar matrix element as well as in the sum rules for the matrix elements of electromagnet current and axial vector current [2–9]. As discussed extensively in Ref. [6], the different asymptotic behavior of various sum rules can be traced to the fact that even and odd parity states contribute with different sign and kinematical factors. If chiral symmetry is realized in the Wigner-Weyl mode at high energies, i.e., by parity doubling, it is possible to have either cancellation or reinforcement between excited state contributions. Irrespective of the exact manner in which these cancellations take place, it is clear that the sum rule in which the continuum contributions are weak is more reliable. This is the case for the chiral-odd sum rule Eq. (2.29), where the continuum factor E_0 appears, to be contrasted with the chiral-even sum rule Eq. (2.30), where the factor E_2 occurs.

Let us now consider the effect of varying χ , which as we have seen earlier is not precisely known. We find that the quality of the overlap of the two sides of the chiral-odd sum rule remains good (as measured by δ) as we change the value of χ, and gets better as χ increases and worse as χ decreases. We also find that the continuum contribution gets larger as χ decreases and smaller as χ increases. For χ values in the range $1.4\,\mathrm{GeV}^{-1} \leq \chi \leq 3.0\,\mathrm{GeV}^{-1}$, we find

$$H = 0.32 - 0.76\ . \tag{2.34}$$

For $\chi < 1.4\,\mathrm{GeV}^{-1}$, we find that the continuum contribution is larger than 50%. This implies that the sum rule is dominated by continuum and the predictions are not reliable for χ values smaller than $1.4\,\mathrm{GeV}^{-1}$.

III. THE NEUTRON-PROTON MASS DIFFERENCE

In this section we consider the relation between the matrix element evaluated in the last section and the neutron-proton mass difference. First let us disregard electromagnetism and work to the first order in the quark mass difference $m_d - m_u$.

Consider the quark mass term in the QCD Hamiltonian density $\mathcal{H}_{\rm QCD}$, as given by

$$\begin{aligned} \mathcal{H}\text{mass} &= m_u\overline{u}u + m_d\overline{d}d + m_s\overline{s}s + \cdots \\ &= \hat{m}(\overline{u}u + \overline{d}d) - \frac{1}{2}\delta m(\overline{u}u - \overline{d}d) + m_s\overline{s}s + \cdots \ . \end{aligned} \tag{3.1}$$

The isospin symmetry is explicitly broken by the term proportional to δm. Using covariant normalization for the hadron state labeled by h and momentum k

$$\langle k', h \mid k, h\rangle \quad = \quad (2\pi)^3 k^0 \delta^{(3)}(\vec{k}' - \vec{k}) \ , \tag{3.2}$$

and regarding the δm term in Eq. (3.1) as a small parameter, we can make a perturbation expansion and write the shift in the mass M_h of the hadron as [10]

$$\delta(M_h) = \frac{-\delta m}{2} \frac{\langle h|(\overline{u}u - \overline{d}d)|h\rangle}{2M_h} \ . \tag{3.3}$$

The matrix element occurring in Eq. (3.3) is to be computed at $\delta m = 0$, which means isospin can be taken to be exact. We can then write for the difference between the neutron and proton mass to first order in δm as

$$(M_n - M_p)_q = \delta m \frac{\langle p|\overline{u}u - \overline{d}d|p\rangle}{2M_p} \ . \tag{3.4}$$

The subscript q in the left-hand side denotes the fact that we are considering only the non-electromagnetic part of the mass difference.

The effect of turning on electromagnetism is described by an effective Lagrangian

$$\mathcal{L}_{\rm e.m.} \quad = \quad -\frac{1}{2}e^2 \int d^4y D(x-y) T j^\mu(x) j_\mu(y) \ , \tag{3.5}$$

where $D(x) = [i4\pi^2(z^2 - i\epsilon)]^{-1}$ is the photon propagator and $j^\mu(x)$ is the electromagnetic current. To remove the divergence arising from electromagnetism one must add counter terms, and these, of course, depend on renormalization prescription. However, this dependence is extremely weak. For example the change in the up quark mass due to a change in the renormalization scale by a factor of two is less than 0.01 MeV. It is therefore meaningful to separate the contribution from the quark mass difference, from that due to electromagnetism. The latter is estimated to be [10]

$$(M_n - M_p)_{\rm elec} = -0.76 \pm 0.30 \ . \tag{3.6}$$

The experimental mass difference is 1.29 MeV, which then gives

$$(M_n - M_p)_q^{\rm exp} = 2.05 \pm 0.30\ . \tag{3.7}$$

In the last section we saw that uncertainty in our knowledge of χ leads to a corresponding uncertainty in our determination of H. For the χ value obtained from chiral perturbation theory [see Eq. (2.23)], we get $(M_n - M_p)_q \simeq 1.8\,\mathrm{MeV}$.

For χ values in the range $2.15\,\mathrm{GeV}^{-1} \le \chi \le 2.80\,\mathrm{GeV}^{-1}$, we find

$$1.75\mathrm{MeV} \le (M_n - M_p)_q \le 2.35\mathrm{MeV}\,, \tag{3.8}$$

which is consistent with experimental data. Smaller and larger values of χ outside the range considered above lead to correspondingly smaller and larger values for the neutron-proton mass difference.

IV. DISCUSSION

One of our main objectives in this paper has been to extract the proton matrix element $H = \langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$. We have seen that the chiral-odd sum rule Eq. (2.29) is reliable for determining this matrix element. The major limiting factor has been the uncertainty in the value of the susceptibility χ. A more accurate evaluation of the two point function Eq. (2.8) should reduce the uncertainty in the value of χ and hence help to pin down the value of the matrix element H.

We also saw that the non-electromagnetic part of the neutron-proton mass difference is essentially given by the matrix element H multiplied by the light quark mass difference δm. If we use a median value $\delta m = 3.3$ MeV and $H \simeq 0.54$ as obtained using a value of $\chi = 2.2\mathrm{GeV}^{-1}$ we get $(M_n - M_p)_q \simeq 1.8\,\mathrm{MeV}$, which indeed has the right sign and magnitude. This suggest that our approach to extract H and the neutron-proton mass difference is reliable. However, since χ and δm are not precisely known we cannot make a critical comparison with data at present.

We now turn to a comparison of our method with those of earlier authors. The nucleon mass was originally extracted by Ioffe [15] with a *combined* use of both the chiral-odd and chiral-even mass sum rules. It is necessary to use these two sum rules together since one must eliminate the coupling constant λ_N^2. Belyaev and Ioffe [16] extended this method to determine the mass splitting between hyperon and nucleon by treating the strange quark mass as a perturbation. In addition to the mass shift, $M_Y - M_N$, one must also take into account the change in the coupling constant $\lambda_Y^2 - \lambda_N^2$ and the change in the continuum threshold s_0. The authors of Refs. [13,14] used the same procedure to determine the mass splittings within an isospin multiplet by treating m_d and m_u as perturbation parameters. In Ref. [11] the neutron-proton mass was extracted directly from the difference between the neutron and proton mass sum rules, but the continuum contributions were disregarded. In Ref. [13], Adami *et.al.* retained continuum corrections but regarded γ as a parameter to be determined by a fit to all isospin splittings in the baryon octet. In Ref. [12], apart from the perturbation due to the quark masses, an attempt was made to incorporate the electromagnetic contribution also phenomenologically in the sum rules.

The sum rules derived by us in Sec. II can also be derived directly from the mass sum rules. Writing $m_u = \hat{m} - \delta m/2$, $m_d = \hat{m} + \delta m/2$ and using $\chi = -\gamma/\delta m$ one can differentiate

Eqs. (16) and (17) of Ref. [12] with respect to δm. One can then identify our sum rules Eqs. (2.29) and (2.30) with Eqs. (29) and (30) of Ref. [12]. (An assumption about the mixed chiral condensate, equivalent to our assumption, $\chi_m = \chi$, was made in Ref. [12]). This coincidence between the sum rules is not surprising, since the quark mass term in the QCD Lagrangian can also be regarded as a constant external scalar field. The double pole term in the RHS of our sum rules clearly arises from the simple pole term in the mass sum rules after the differentiation of the proton mass with respect to δm.

We note that the term proportional to the mixed quark-gluon condensate [the fourth term in the LHS of our Eq. (2.29)] has not been included in Ref. [13]. We have seen in our analysis of the sum rules (see Fig.2) that this term is numerically significant. There is also a minor discrepancy in the coefficient of the four-quark condensate term between Ref. [13] and this work (or Ref. [12]). This discrepancy comes from the fact that the authors of Ref. [13] directly used the Σ and Ξ mass sum rules from Ref. [16], where *not* all the quark mass terms were taken into account.

It is now easy to see, as discussed earlier in Sec. II, why Eq. (2.29) is a better sum rule as compared to the chiral-even sum rule Eq. (2.30). In the chiral-odd sum rule, the perturbation due to the finite quark mass does not affect the leading asymptotic behavior and hence when a differentiation with respect to δm (alternately when the neutron and proton sum rule difference is taken) the leading asymptotic behavior reduces to a smaller power of the Borel Mass M^2, which in turn means weaker dependence on the continuum contribution. On the other hand, in the chiral-even sum rule the introduction of quark mass leads to the term $m_d M^6$ in the proton and $m_u M^6$ in the neutron sum rule. Consequently in the difference the leading asymptotic behavior is now M^6. In other words, the continuum contributions are enhanced. This feature is also clearly reflected in our analysis in Sec. II. For the chiral-odd sum rule the double pole term residue was stable when s_0 was varied while in the chiral-even sum rule the corresponding residue was unstable. Further, in the chiral-even sum rule the single pole term corresponding to transition between proton and the excited states dominated over the double pole term. We would also like to point out that inclusion of instanton contributions improves the chiral-even mass sum rule [31]. In the light of our observations above regarding the relation of our sum rules to the mass sum rules it suggests that such instanton contributions can also be significant in our sum rule Eq. (2.30).

It is also worth emphasizing that in our work two stages are involved. We first calculate a hadronic matrix element H. This involves the susceptibility χ, which being essentially the ratio $-\gamma/\delta m$ is relatively insensitive to errors in our knowledge of δm. The quark mass part of the neutron-proton mass difference was obtained as the product $H\delta m$.

As a final remark we shall comment on the Nolen-Schiffer anomaly [32]. We saw in the last section that the empirical neutron-proton mass difference can be written as

$$(M_n - M_p)^{\rm exp} \quad = -0.76 + \delta m H \ . \tag{4.1}$$

Now, it is well known that the matrix element of the axial vector current is quenched [33] inside the nuclear medium by about 30 percent. It may be reasonable to assume that the isovector-scalar matrix element $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$ is also quenched in a similar fashion.

Assuming then for example a 30 percent reduction in the value of H, it follows form Eq. (4.1) that the effective mass difference in the nuclear medium is $(M_n - M_p)^{\rm exp}_{\rm med} \simeq$

0.49 MeV. Understanding the Nolen-Schiffer anomaly is then reduced to explain the quenching of $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p$ in nuclear medium. This can be handled either by traditional nuclear structure calculations or again by use of QCD sum rules as in the quenching of nucleon axial coupling [34,35].

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FIGURES

FIG. 1. Diagrams for the calculation of the Wilson coefficients of the correlation function. The solid, wavy and dashed lines represent the quark, gluon, and external field, respectively.

FIG. 2. Borel mass dependence of the left-hand side (solid curve) and right-hand side (long-dashed curve) of Eq. (2.29), with $\chi = 2.2\,\mathrm{GeV}^{-1}$ and the optimized values $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p = 0.54$ and $\tilde{A}_q = 0.29\,\mathrm{GeV}^5$. The curves 1, 2, 3 and 4 correspond to the first, second, third and fourth terms in the LHS of Eq. (2.29).

FIG. 3. Borel mass dependence of the left-hand side (solid curve) and right-hand side (long-dashed curve) of Eq. (2.30), with $\chi = 2.2\,\mathrm{GeV}^{-1}$ and the optimized values $\langle p|\overline{u}u - \overline{d}d|p\rangle/2M_p = 0.01$ and $\tilde{A}_1 = -1.82\,\mathrm{GeV}^6$. The curves 1, 2 and 3 correspond to the first, second and third terms in the LHS of Eq. (2.30).