Isospin breaking and instantons in QCD nucleon sum rules

Hilmar Forkel

European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Villa Tambosi, Strada delle Tabarelle 286, I-38050 Villazzano, Italy

Marina Nielsen

Instituto de Física, Universidade de São Paulo, Caixa Postal 66318, 05389-970 São Paulo, SP, Brazil

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We study isospin-breaking instanton corrections to the operator product expansion of the nucleon correlation functions. After a comparison with quark model calculations based on the 't Hooft interaction, we examine the role of instantons in the corresponding QCD sum rules. Instanton contributions are found to be absent in the chirally even sum rule, but significant in the chirally odd one. They improve the consistency of both sum rules and favor a value of the isovector quark condensate close to the chiral estimate. [S0556-2821(97)01003-5]

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I. INTRODUCTION

Over the last years growing evidence for a significant role of QCD instantons in hadron structure has been collected. It originated first from models built on instanton vacuum phenomenology [1,2] and recently received model-independent support from cooled lattice studies [3]. Indeed, the latter show that hadron correlation functions remain almost unchanged if all but the instanton fields are filtered out of the equilibrated lattice configurations.

Analytical studies of instanton contributions to the operator product expansion (OPE) and to QCD sum rules find a reflection of this picture in the importance of explicit instanton corrections in the pion [4] and nucleon [5] channels. The corrections in the nucleon channel show a characteristic pattern, which originates from the chirality of the quark zero mode states in the instanton background: they are small in the chirally even nucleon correlator and in the corresponding sum rule, but significant in the chirally odd one. Indeed, the chirally odd sum rule could hardly be stabilized without instanton corrections, whereas the chirally even one is stable and in agreement with phenomenology even if the instanton contribution is neglected [6].

An analogous pattern was found in two recent sum rule calculations of the neutron-proton mass difference δM_N [7,8] *without* instanton corrections, which also show a significant discrepancy between the results of the chirally even and odd sum rules. Again, the former agrees well with phenomenology ($\delta M_N \approx 2$ MeV), whereas the latter yields a value consistent with zero and thus puts the consistency of the two sum rules into question.¹ This analogy with the nucleon mass sum rules prompted us to examine instanton corrections to the isospin-violating nucleon sum rules, which is the subject of the present paper.

A further, closely related sum rule calculation of isospin

violation in baryons without instanton corrections [9] takes a somewhat different approach. The baryon mass splittings are taken as input from experiment (after subtraction of the estimated electromagnetic contributions), and the two relevant isospin-breaking parameters—the quark mass difference δm and the difference of up- and down-quark condensates γ —are estimated from the sum rules. This analysis seems to find consistency between both sum rules, at least if the difference $\delta \lambda_N^2$ between the neutron and proton pole strengths is fitted, and thus seems incompatible with the conclusions of Refs. [7,8]. The fit requires, however, an unusually small value of $|\gamma|$, about a quarter of the one estimated from chiral perturbation theory, and an uncomfortably large continuum contribution. We will come back to this issue below.

The study of isospin violations in QCD nucleon sum rules can be based either on the nucleon correlator in an iospinviolating scalar background field [8] or on the difference of the neutron and proton correlators [7,9]. We will adopt the latter approach. In Sec. II we calculate the leading, isospinviolating instanton corrections to the nucleon correlator, and in Sec. III we discuss their structure in more detail. Section IV contains a comparison with quark model calculations based on instanton-induced interactions. We point out, in particular, that the neglect of the vacuum sector in many of these models leads to severe limitations in their description of isopin violation effects. On the basis of the instantoncorrected nucleon correlators from Sec. II we then set up the correponding QCD sum rule in Sec. V and analyze it quantitatively in Sec. VI. The final section contains a summary of our results and some conclusions.

II. NUCLEON CORRELATORS

This section describes the evaluation of small-scale instanton contributions to the nucleon correlators in the presence of isopin breaking. We begin with the correlation function in the proton channel, which is characterized by two invariant amplitudes of opposite chirality:

$$\Pi_{p}(q) = i \int d^{4}x e^{iq \cdot x} \langle 0 | \mathrm{T} \eta_{p}(x) \overline{\eta}_{p}(0) | 0 \rangle$$
$$= \langle q \Pi_{q,p}(q^{2}) + \Pi_{1,p}(q^{2}).$$
(1)

¹Attempts to reduce this discrepancy by adding a term attributed to electromagnetic corrections to the OPE [7] would require a substantial corresponding refinement on the phenomenological side of the sum rule, see Ref. [9].

The composite operator η_p is built from QCD fields and serves as an interpolating field for the proton. Two such (independent) operators with minimal mass dimension (i.e., 9/2) can be constructed. We adopt the standard choice of Ioffe [6]:

$$\eta_p(x) = \epsilon_{abc} [u_a^T(x) C \gamma_\mu u_b(x)] \gamma_5 \gamma^\mu d_c(x)$$
(2)

(the neutron current is obtained by interchanging up- and down-quark fields), which allows for a direct comparison with the previous studies of isospin violation in nucleon sum rules [7-9].

The leading instanton contributions to the correlators can be calculated in the semiclassical approximation, i.e., by evaluating Eq. (1) in the background of the instanton field and by taking the weighted average of the resulting expression over the quantum distribution of the instanton's collective coordinates [5]. These contributions add nonperturbative corrections to the Wilson coefficients of the conventional OPE, with which they will be combined in Sec. V. Isospin breaking originates in this framework from the mass difference of up and down quarks,

$$\delta m = m_d - m_u, \qquad (3)$$

and from the differences in the values of the corresponding condensates,

$$\gamma \equiv \frac{\langle 0|dd - \overline{u}u|0\rangle}{\langle 0|\overline{u}u|0\rangle}.$$
(4)

The isovector quark condensate, which determines γ , is the dominant source of nonperturbative isospin violation in the OPE of the correlators, since it originates from the lowest-dimensional operators with a finite vacuum expectation value. The value of γ has been estimated in a variety of approaches [9–16], with results varying over almost an order of magnitude, $-1 \times 10^{-2} \leq \gamma \leq -2 \times 10^{-3}$. The sensitivity of the baryon sum rule analysis to γ can be used for an additional estimate of its value [9], which will be adapted to the presence of instanton corrections in Sec. VI. For the quark mass difference we use the more accurately known standard value $\delta m = 3.3$ MeV [10].

The rationale behind the semiclassical treatment of instanton contributions and the calculational strategy are analogous to those in the isosymmetric case [5], and we thus just sketch the essential steps here. To leading order in the product of quark masses and instanton size, instanton effects in the nucleon correlators are associated with the quark zero modes [17]

$$\psi_0^{\pm}(x) = \frac{\rho}{\pi} \frac{1 \pm \gamma_5}{(r^2 + \rho^2)^{3/2}} \frac{r}{r} U,$$
(5)

where the superscript \pm corresponds to an (anti-) instanton of size ρ with center at x_0 . The spin-color matrix U satisfies $(\vec{\sigma} + \vec{\tau})U = 0$ and $r = x - x_0$. The zero mode contributions enter the calculation of the correlators through the leading term in the spectral representation of the quark background field propagator:

$$S_{q}^{\pm}(x,y) = \frac{\psi_{0}^{\pm}(x)\psi_{0}^{\pm\dagger}(y)}{m_{a}^{*}(\rho)} + O(\rho m_{q}^{*}).$$
(6)

The flavor-dependent effective quark mass $m_q^*(\rho) = m_q - 2/3\pi^2 \rho^2 \langle \bar{q}q \rangle$ (where q stands for up or down quarks) in the denominator is generated by interactions with long-wavelength QCD vacuum fields [18]. Quark propagation in the higher-lying continuum modes in the instanton background will be approximated as in [5] by the free quark propagator.

Note that both the zero and continuum mode propagators are flavor dependent. The zero mode part contains the effective quark mass, which depends on the current quark masses and on the corresponding condensates. The current quark masses enter, of course, also the continuum mode contributions.

With the quark background field propagator at hand, the instanton contributions to the proton and neutron correlators can now be evaluated. As a first, generic result we find that the chirally even amplitudes Π_q for both proton and neutron do not receive leading instanton corrections. This generalizes the analogous observation in Ref. [5] to finite current quark masses and condensate differences and is a consequence of using Ioffe's current. The isopin-breaking difference of the Π_q 's for neutron and proton, moreover, vanishes for *all* interpolating fields, as we will show in the next section.

The chirally odd amplitudes Π_1 , on the other hand, get sizable instanton contributions, and their difference for proton and neutron remains finite. For the proton correlator, to first order in the current quark masses and continued to Euclidean space-time, we obtain

$$\Pi_{1,p}^{\text{inst}}(q^{2}) = -\frac{16}{\pi^{4}} \int d\rho \rho^{4} \frac{n(\rho)}{m_{0}^{*2}(\rho)} \int d^{4}x e^{iqx} \\ \times \left(\frac{1-\zeta}{N_{c}} \langle \overline{u}u \rangle - \frac{im_{u}}{\pi^{2}x^{2}} \right) \int d^{4}x_{0} \\ \times \frac{1}{[(x-x_{0})^{2} + \rho^{2}]^{3} [x_{0}^{2} + \rho^{2}]^{3}}, \qquad (7)$$

where N_c is the number of quark colors. The isoscalar part of the effective quark mass in the chiral limit is defined as $m_0^*(\rho) = -\frac{2}{3}\pi^2 \rho^2 \langle \bar{q}q \rangle_0$ with $\langle \bar{q}q \rangle_0 \equiv (\langle \bar{u}u \rangle + \langle \bar{d}d \rangle)/2$ and the dimensionless ratio $\zeta = (m_u + m_d)/m_0^*$.

The further evaluation of Eq. (7) requires an explicit expression for the instanton size distribution $n(\rho)$ in the vacuum. Instanton liquid vacuum models [19] and the analysis of cooled lattice configurations [3] have produced a consistent picture of this distribution. The sharply peaked, almost Gaussian shape of $n(\rho)$ found in Ref. [19] can be sufficiently well approximated as [20]

$$n(\rho) = \overline{n} \,\delta(\rho - \overline{\rho}), \quad \overline{n} \simeq \frac{1}{2} \text{ fm}^{-4}, \quad \overline{\rho} \simeq \frac{1}{3} \text{ fm}, \quad (8)$$

which neglects the small half width (≈ 0.1 fm) of the distribution. In Eq. (8) we introduced the average instanton size $\overline{\rho}$ and the instanton number density \overline{n} , which equals the density of anti-instantons. \overline{n} can be approximately related [21] to

the isoscalar quark condensate by the self-consistency condition $\overline{n} = -\frac{1}{2}m_0^*(\overline{\rho})\langle \overline{q}q \rangle_0$, which quite closely reproduces the phenomenological value given above and allows the elimination of \overline{n} in favor of the quark condensate.

After performing the now trivial integration over instanton sizes, we prepare the amplitude (7) for its use in the corresponding sum rule by applying the standard Borel transform [22],

$$\Pi(M^2) \equiv \lim_{n \to \infty} \frac{1}{n!} (Q^2)^{n+1} \left(-\frac{d}{dQ^2} \right)^n \Pi(Q^2)$$
(9)

 $(Q^2 = -q^2)$ with the squared Borel mass scale $M^2 = Q^2/n$ kept fixed in the limit, and obtain

$$\Pi_{1,p}^{\text{inst}}(M^2) = -\frac{3}{4\pi^2} \bigg[\frac{1-\zeta}{N_c} \langle \bar{u}\bar{u} \rangle M^4 I_1(M^2 \bar{\rho}^2) \\ -\frac{1}{16\pi^2} m_u \bar{\rho}^4 M^{10} I_2(M^2 \bar{\rho}^2) \bigg], \qquad (10)$$

in terms of the two dimensionless integrals

$$I_1(z^2) = \int_{z^2/4}^{\infty} dx \, \frac{x^2}{(x - z^2/4)^2} e^{-x^2(x - z^2/4)^{-1}}, \qquad (11)$$

$$I_{2}(z^{2}) = \int_{0}^{\infty} dx_{1} \int_{0}^{z^{-2}} dx_{2} \frac{x_{2}^{2}(z^{-2} - x_{2})^{2}}{(x_{1} + x_{2} - z^{2}x_{2}^{2})^{5}} \\ \times \exp\left[-\frac{1}{4}(x_{1} + x_{2} - z^{2}x_{2}^{2})^{-1}\right].$$
(12)

The amplitude for the neutron follows from Eq. (10) by interchanging up- and down-quark masses and condensates. Equation (10) generalizes the isospin-symmetric amplitude of Ref. [5], which is recovered in the chiral limit.

The two integrals (11) and (12) contain the instanton corrections to the Borel-transformed Wilson coefficients of the unit operator (in I_2) and of $\langle \overline{uu} \rangle$ (in I_1). Additional contributions from quark modes with momenta below the renormalization scale μ of the OPE should be excluded from I_1 and I_2 in order to avoid double counting of the physics contained in the condensates. Fortunately, the instanton background field induces only one soft contribution up to operators of dimension 6, corresponding to a four-quark condensate in I_2 . We will correct for this contribution in Sec. V.

III. ISOPIN VIOLATION AND INSTANTONS

It is instructive to analyze the isospin properties and the origin of isospin breaking in the instanton induced amplitude (10) in more detail. This analysis will also lay the foundation for our discussion in the next section, where we clarify some crucial differences between our approach and quark model calculations. These differences explain, in particular, the absence of instanton-induced contributions to δM_N in many quark models, contrary to our findings in the correlator approach.

The gluonic sector and the quark-gluon vertex of QCD are both flavor independent. The structure of the interaction

with the instanton background field is thus the same for up and down quarks and the background field propagator (6) is diagonal in isopin space. Its only flavor dependence enters through the current quark masses and condensates in m_q^* . This has characteristic consequences for the instantoninduced interactions between quarks, which generate the correlator amplitude (10) and can be extracted from the calculation in Sec. II:

$$\langle 0|Tq_{A,\alpha,a}(x_1)\overline{q}_{B,\beta,b}(y_1)q_{C,\gamma,c}(x_2)\overline{q}_{D,\delta,d}(y_2)|0\rangle$$

= $(\delta_{AB}\delta_{CD} - \delta_{AD}\delta_{CB})\int d\rho \frac{n(\rho)}{(m_u^*\rho)(m_d^*\rho)}(2\pi^2\rho^3)^2$
 $\times \int d^4x_0C(r_1)C(u_1)C(r_2)C(u_2)$
 $\times \sum_{L/R} \langle \langle (P_{L/R}\widetilde{P}_{ab})_{\alpha\beta}(P_{L/R}\widetilde{P}_{cd})_{\gamma\delta} \rangle \rangle_{\mathrm{SU}(3)_c}.$ (13)

In this expression, capital Latin, Greek, and small Latin indices refer to isospin, Dirac spin, and color, respectively. The angular brackets indicate the average of the instanton's color orientation over the Haar measure of SU(3)_c. The chiral projection operators are $P_{L/R} = (1 \pm \gamma_5)/2$, the distances from the instanton center are denoted $r_i = \sqrt{(x_i - x_0)^2}$ and $u_i = \sqrt{(y_i - x_0)^2}$, the nonlocality of the vertex is contained in the functions

$$C(r) = \left(\frac{r^2}{r^2 + \rho^2}\right)^{3/2},$$
 (14)

and its color structure is given by the spin-color tensor

$$\widetilde{P}_{\alpha\beta,ab} = \delta_{\alpha\beta} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}_{ab} - \vec{\Sigma}_{\alpha\beta} \begin{pmatrix} \vec{\tau} & 0 \\ 0 & 0 \end{pmatrix}_{ab}, \quad (15)$$

which makes the embedding into an SU(2) subgroup of $SU(3)_c$ explicit and contains the characteristic spin-color coupling. Lorentz and color covariance become manifest only after averaging over the color group.

The nonlocal four-quark vertex (13) originates from the quark zero modes in the instanton field and was first derived by 't Hooft [17] for $m_q^* = m_q$. It has, separately for both quark chiralities, a well-known determinantal flavor structure and is thus $SU(2)_L \times SU(2)_R$ and, in particular, isospin symmetric.² Even if the flavor-dependent quark masses and condensates enter the vertex explicitly, isospin violation thus cannot originate solely from the instanton-induced interaction. In the OPE, however, this vertex generates nonperturbative contributions to the Wilson coefficients, which can either themselves become isopin violating due to the finite quark mass difference or multiply isopin violating operators. Examples for both of these cases were found in Sec. II.

²In addition, it breaks the axial $U_A(1)$ symmetry, which is a reflection of the Adler-Bell-Jackiw anomaly and a celebrated instanton effect [17].

At short distances, multi-instanton contributions to the nucleon correlators are suppressed since $x/\overline{R} \ll 1$. Additional corrections, which originate from only one valence quark propagating in a zero mode state and generate contributions to the quark self-energy, are subleading in $m^*\overline{\rho}$ and not considered in this paper.

The structure of the instanton-induced four-point function (13) explains some qualitative features of the correlator (10). The definite chirality of the quark legs, inherited from the zero mode states, lets this vertex act only between quarks which are coupled to spin 0 in the interpolating fields, and the Dirac structure of the instanton contribution to the nucleon correlator is thus determined by the remaining "valence" quark line. Only the contribution to the Wilson coefficient of the unit operator, in which this line is in a nonzero-mode state (approximated by the free quark propagator), can thus generate a chirally even amplitude. According to our discussion above, however, such contributions are isospin conserving and this explains why the difference of the chirally even amplitudes of the neutron and proton correlators is not corrected by instantons for any choice of the interpolating field. The instanton contributions to the chirally even amplitudes of neutron and proton vanish individually only for the Ioffe current, as already pointed out.

Another characteristic feature of the correlator (10) follows directly from the flavor structure of the 't Hooft vertex. Since only one quark pair of each flavor can take part in the zero-mode induced interaction (13), the valence quark in the non-zero-mode state in the proton (neutron) correlator must be an up (down) quark. This explains why we find only contributions proportional to the up-quark mass and condensate in Eq. (10).

To summarize, instanton-induced interactions contribute to isopin breaking in the operator product expansion of the nucleon correlators (in the framework of our approximations) in two distinct ways: they correct the Wilson coefficient of the unit operator, which becomes isopin dependent due to the difference of the current quark masses, and they contribute to the coefficients of the isospin-violating operators \overline{uu} and \overline{dd} . Both of these corrections affect only the chirally odd amplitude of the correlators.

IV. COMPARISON WITH QUARK MODELS

Instanton-induced interactions have been included in several quark model calculations of mass splittings in baryon isomultiplets. It is useful to compare the results of such calculations to those of our approach. To be specific, we will base this comparison on studies in the MIT bag model [23,24], which deals with relativistic, light quarks and is in this respect similar to the correlator approach. Most of our conclusions, though, will apply to a wider range of quark models.

Bag model calculations of hadron mass shifts because of instantons [25] are based on a localized version of the 't Hooft interaction, cast into the form of an effective Lagrangian. Indeed, the pointlike limit of the vertex (13) (in Minkowski space) is reproduced by the Lagrangian [18]

$$\mathcal{L}_{\text{inst}} = -\left(\frac{4}{3}\pi^{2}\bar{\rho}^{3}\right)^{2}\frac{\bar{n}}{(m_{u}^{*}\bar{\rho})(m_{d}^{*}\bar{\rho})}\sum_{L/R}\left\{(\bar{u}_{R}u_{L})(\bar{d}_{R}d_{L}) + \frac{3}{32}\left[(\bar{u}_{R}\lambda_{a}u_{L})(\bar{d}_{R}\lambda_{a}d_{L}) - \frac{3}{4}(\bar{u}_{R}\lambda_{a}\sigma_{\mu\nu}u_{L}) \times (\bar{d}_{R}\lambda_{a}\sigma^{\mu\nu}d_{L})\right]\right\},$$
(16)

which is obtained from Eq. (13) by amputating the external quark propagators, neglecting the nonlocality due to the finite instanton size, performing the average over the color orientation of the instanton,³ specifying the instanton density in the form (8) and continuing back to Minkowski spacetime.

The shrinking of the instanton vertex to its pointlike limit will probably not cause significant errors in bag model results for low-lying hadrons. This is because quarks in the bag can separate up to the diameter $2R \sim 2$ fm, so that their inverse momenta in the ground state are considerably larger than the average instanton size which characterizes the extent of the vertex. Note, however, that the nucleon correlator in QCD sum rule calculations is probed at an order of magnitude smaller distances, where the details of the short-distance dynamics and thus the nonlocality of the vertex become important.

In addition to the structure of the instanton-induced quark interaction, bag calculations share some other common features with the nucleon correlators (1), notably in the construction of the nucleon states. The spin, color, and flavor structure of the bag model [i.e., SU(6)] proton state,

$$|p,\uparrow\rangle = \frac{1}{\sqrt{18}} \epsilon_{abc} [(u_{a\downarrow}^+ d_{b\uparrow}^+ - u_{a\uparrow}^+ d_{b\downarrow}^+) u_{c\uparrow}^+]|0\rangle.$$
(17)

[arrows indicate the value of the total spin projection j_3 of the quarks (in the bag ground state) and of the proton] and the corresponding one for the neutron (which are obtained from $-|p\rangle$ by interchanging up and down quarks) are essentially identical to that of the interpolators (2). This is, of course, just a consequence of the fact that both are constructed to carry nucleon quantum numbers, which ensures that they have identical properties under Lorentz, color, isospin, and the standard discrete transformations.

Despite these similarities, bag model calculations do not find any instanton contribution to the proton-neutron mass difference⁴ [23,24]. The neutron and proton mass shifts induced by Eq. (16) are evaluated in first order perturbation theory between the SU(6) states. A straightforward calculation gives

³As long as this Lagrangian is evaluated only in color singlet states, one could, of course, skip the color averaging and use the neither Lorentz nor $SU(3)_c$ -invariant version instead, with identical results.

⁴As long as one-zero-mode corrections (see above) are neglected.

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$$\left\langle p \right| - \int d^{3}x \mathcal{L}_{\text{inst}}(x) \left| p \right\rangle$$

$$= \left(\frac{4}{3} \pi^{2} \overline{\rho}^{3} \right)^{2} \frac{\overline{n}}{(m_{u}^{*} \overline{\rho})(m_{d}^{*} \overline{\rho})} \left(\frac{N_{u} N_{d}}{8 \pi} \right)^{2}$$

$$\times \int d^{3}x \{ 5 (a_{1}^{2} - a_{2}^{2})^{(u)} (a_{1}^{2} - a_{2}^{2})^{(d)}$$

$$+ 4 (a_{1}^{2} + a_{2}^{2})^{(u)} (a_{1}^{2} + a_{2}^{2})^{(d)} + 20 a_{1}^{(u)} a_{2}^{(u)} a_{1}^{(d)} a_{2}^{(d)} \}$$

$$(18)$$

(the integrations extend over the bag volume) where the ground state quark wave function in the bag is written as

$$\psi_{j_3}^{(q)} = \frac{N_q}{\sqrt{4\,\pi}} \begin{pmatrix} a_1^{(q)}(r) \\ i\,\vec{\sigma}\,\vec{r}\,a_2^{(q)}(r) \end{pmatrix} \chi_{j_3},\tag{19}$$

with $a_1^{(q)} = \sqrt{(\omega_q + m_q)/\omega_q} j_0(\kappa_q r/R)$ and $a_2^{(q)} = \sqrt{(\omega_q - m_q)/\omega_q} j_1(\kappa_q r/R)$. [*R* is the bag radius, N_q a normalization constant, χ_{j_3} are the Pauli spinors, and ω_q , κ_q are the energy and (dimensionless) momentum quantum numbers of the quark ground state.] The result for the neutron matrix element can be immediately inferred from Eq. (18) by exchanging up- and down-quark operators in the proton states. Since \mathcal{L}_{inst} is symmetric under $u \leftrightarrow d$, one can as well exchange *u* and *d* everywhere in the expression for the proton matrix element. Equation (18), however, is manifestly invariant under this exchange and, therefore, the difference of the matrix elements indeed vanishes:

$$\delta M_{N,\text{bag}}^{\text{inst}} = \left\langle p \left| \int d^3 x \mathcal{L}_{\text{inst}} \right| p \right\rangle - \left\langle n \left| \int d^3 x \mathcal{L}_{\text{inst}} \right| n \right\rangle = 0.$$
(20)

This is in contrast with the result for the Boreltransformed nucleon correlators:

$$\Pi_{1,n}^{\text{inst}}(M^2) - \Pi_{1,p}^{\text{inst}}(M^2) \neq 0, \qquad (21)$$

which can be translated via a QCD sum rule into a finite instanton contribution to the mass difference (see below).

Of course, the bag model contains *ad hoc* assumptions on quark confinement, breaks chiral symmetry explicitly, and differs also in other aspects from the model-independent correlator approach. One would thus not expect the results to agree quantitatively. It is at first surprising, however, to find a qualitative difference, namely, the exact absence of *any* instanton-mediated mass shift $\delta M_{N,\text{bag}}^{\text{inst}}$. In view of the similarity of the interactions (13) and (16) one is led to search for the origin of this difference in the description of the nucleon states. And indeed, here, the two approaches differ crucially.

A first difference is that the quarks in the bag matrix elements are restricted to their ground states with total spin j=1/2 (i.e., to l=0 or 1), whereas the interpolators can create quarks in all orbital angular momentum states. In fact, the created pointlike wave packet has overlap with the whole tower of excited states carrying nucleon quantum numbers, including states in the many-particle continuum. Experience from QCD sum rules [6] and from lattice data [26,27] shows,

however, that already at rather small distances a main contribution to the nucleon correlator comes from the nucleon ground state. This tendency is further enhanced by the Borel transform, which exponentially suppresses contributions from higher-lying states. One does therefore not expect these states to contribute significantly to a finite value of the difference (21) in the fiducial Borel mass domain (see below), let alone to be its only cause.

Indeed, the crucial difference between the bag and correlator results can rather be traced to the description of the nucleon ground states themselves, and in particular to their flavor content. While the SU(6) states (17) [as well as the interpolating fields (2)] have good isospin, this is *not* the case for the states $\eta_{p,n}|0\rangle$ which are created by the interpolators and studied in the correlator (1).

Virtual "sea" quarks and other perturbative and nonperturbative vacuum fluctuations give these states a much richer (and more realistic) flavor structure. They inherit, in particular, isospin-breaking components from the vacuum fields. The short-distance part of this nontrivial flavor content is captured both in the OPE and in the instanton corrections and causes Eq. (21) to be finite. At very short distances it originates from the quark mass differences, and at larger distances it enters predominantly through the difference between up- and down-quark condensates. The neglect of both of these ingredients in the isospin structure of the bag wave functions leads, on the other hand, to the symmetry of the proton matrix element (18) under exchange of the two quark flavors in the states (17) and thus to the absence of an instanton-induced mass difference, Eq. (20).

In Ref. [24] an attempt was made to include longwavelength vacuum fields into the bag interior. Long- and short-distance physics inside the bag, however, cannot be reliably separated. In particular, such a scale separation (which is indispensable to control the interactions with the vacuum fields) cannot be based on a short-distance expansion, which would, in fact, badly diverge at distances of the order of the bag radius $R \sim \Lambda_{\rm QCD}^{-1}$. Higher order interactions with the background fields (leading to contributions from higher-dimensional condensates) are thus not suppressed, and it is difficult to see how their neglect can be justified and how double counting of quark physics can be avoided. In addition, both the contributions of the interactions with the long-wavelength background fields and with the instanton to the matrix elements are calculated independently to leading order and then added. Combined effects of instantons and the other vacuum fields, as described by the OPE, are therefore still lacking⁵ and Eq. (20) remains to hold.

The large-distance scales over which quarks can interact are a generic bag model problem, since clearly, not all nonperturbative physics can be absorbed into the boundary conditions. For QCD sum rule calculations, on the other hand, a reliable description of the correlation functions up to distances of about 0.2 fm is usually sufficient. At these rather small distances the long-wavelength physics can still be con-

⁵Except for the factor $(m_u^* m_d^*)^{-1}$ in the instanton-induced interaction (16).

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trolled in a model-independent way by only a few generic and physical parameters, the low-dimensional condensates.

Instanton physics supplies, in fact, yet another example for the problems with treating quark interactions in the large bag interior. The neglect of multi-instanton effects (beyond the mean field level) is a basic assumption underlying the interactions (13) and (16). This approximation can be justified in the correlator for distances $x \ll \overline{R}$, but hardly at the scales set by the bag diameter. Instanton liquid simulations [28] indeed confirm that multi-instanton effects become important at distances of the order of the average separation between instantons, $x \ge \overline{R} \simeq 1$ fm.

To conclude, quark and bag model calculations that restrict the evaluation of instanton-induced baryon mass shifts to calculating the expectation value of the effective 't Hooft Lagrangian between SU(6) eigenstates miss important sources of isospin asymmetry, in particular from isospinviolating vacuum fields. This physics, which significantly affects the estimates of mass splittings in baryon isomultiplets, is, however, captured in the instanton-corrected OPE of the nucleon correlators.

V. ISOPIN-VIOLATING NUCLEON SUM RULES

In this section we combine the instanton contributions to the nucleon correlation functions with the conventional operator product expansion [7] and set up the QCD sum rule for the difference of the neutron and proton correlators.

Since the average instanton size $\overline{\rho}$ is smaller than the inverse renormalization point $\mu^{-1} \simeq 0.4$ fm of the OPE, the major part of the instanton corrections will contribute to the Wilson coefficients. These corrections can be directly added to the standard OPE, since they originate from nonperturbative physics which was not previously accounted for.

The integral I_2 in Eq. (10), however, contains in addition to the instanton contribution to the Wilson coefficient of the unit operator also a soft part, as pointed out in Sec. II. It originates from the region in loop momentum space where the hard external momentum Q^2 is carried exclusively by the quark line which is not participating in the zero-mode induced interaction. No such contribution is contained in I_1 , since here the third quark line interacts with the quark condensate and thus does not carry momentum.

The soft part of I_2 represents an instanton contribution to the four-quark condensate. Fortunately, this is the only operator up to dimension 6 which receives such a correction. Indeed, a general theorem [29] severely limits the number of condensates in the OPE of hadronic correlators which can be induced by self-dual background fields.

In order to prevent double counting of long-wavelength physics, the four-quark condensate terms in the OPE and the instanton contributions have to be adapted before combining them with the other OPE terms of Π_1 . As in Ref. [5], we will neglect the comparatively small OPE contribution to $\langle \overline{uudd} \rangle$ and keep instead the contribution induced by the 't Hooft vertex in the limit of vanishing external momenta. A more accurate procedure, namely to subtract explicitly the part of the instanton contribution which originates from momenta below the renormalization scale, will be described elsewhere [30]. Four-quark condensates of the type $\langle \overline{uuu} \rangle$ and $\langle \overline{dddd} \rangle$, on the other hand, do not receive singleinstanton contributions and remain unchanged.

After implementing the above modification, we can combine the instanton part (10) with the OPE of the chirally odd sum rule of Ref. [7]. Taking the difference of the neutron and proton sum rules and transferring the continuum contributions to the left-hand (i.e., OPE) side, we obtain

$$\frac{M^{6} \delta m}{16\pi^{4}} E_{2} L^{-8/9} - \frac{\gamma}{4\pi^{2}} \langle \bar{q}q \rangle_{0} M^{4} E_{1} + \frac{4}{3} \delta m \langle \bar{q}q \rangle_{0}^{2}
+ \frac{\gamma}{4\pi^{2}} \langle \bar{q}q \rangle M^{4} I_{1}(z^{2}) - \frac{3}{64\pi^{4}} \delta m \bar{\rho}^{4} M^{10} I_{2}(z^{2}) L^{-8/9}
= \left[2\lambda_{N}^{2} \frac{M_{N}^{2}}{M^{2}} \delta M_{N} - \lambda_{N}^{2} \delta M_{N} - \delta \lambda_{N}^{2} M_{N} \right] e^{-M_{N}^{2}/M^{2}}
- \frac{1}{4\pi^{2}} \langle \bar{q}q \rangle_{0} s_{1} e^{-s_{1}/M^{2}} \delta s_{1},$$
(22)

where $M_N = (M_p + M_n)/2$ and $\lambda_N = (\lambda_p + \lambda_n)/2$ denote the isoscalar nucleon mass and coupling to the interpolating field. (We neglect the small gluon condensate contribution.) The isospin-violating differences of the overlap and threshold parameters are $\delta \lambda_N^2 = \lambda_n^2 - \lambda_p^2$, $\delta s_1 = s_{1n} - s_{1p}$, and the factor $L^{-8/9}$, with $L = \ln(M^2/\Lambda_{\rm QCD}^2)/\ln(\mu^2/\Lambda_{\rm QCD}^2)$ and $\Lambda_{\rm QCD} = 150$ MeV, accounts for the anomalous dimensions of the composite operators and sets their renormalization point to $\mu = 500$ MeV.

The contributions from the continuum, starting at the effective threshold s_1 , are as usual combined with the leading and described by the functions OPE term $E_1 = 1 - e^{-s_1/M^2} (s_1/M^2 + 1)$ and $E_2 = 1 - e^{-s_1/M^2} (s_1^2/2M^4)$ $+s_1/M^2+1$ [6]. Their definitions are identical to those in the individual sum rules. Note that additional terms in the difference sum rules, proportional to δs_1 and δs_q (see below), originate from the continuum terms of the individual sum rules. They do not correspond to the cut structure (i.e., to the leading OPE behavior) of the difference sum rule, however, and are thus not needed to match the large-s behavior of the OPE.

With the standard definitions $a \equiv -4 \pi^2 \langle \bar{q}q \rangle_0$, and $\tilde{\lambda}_N^2 \equiv 32 \pi^4 \lambda_N^2$, our sum rule equation (22) now assumes its final form

$$e^{M_N^2/M^2} \left[M^8 \,\delta m E_2 L^{-8/9} + M^6 \,\gamma a E_1 + \frac{4}{3} \,\delta m M^2 a^2 - M^6 \,\gamma a I_1(z^2) - \frac{3}{4} \,\delta m \bar{\rho}^4 M^{12} I_2(z^2) L^{-8/9} \right]$$

$$= \tilde{\lambda}_N^2 M_N^2 \,\delta M_N - \left(\frac{\tilde{\lambda}_N^2}{2} \,\delta M_N + \frac{\delta \tilde{\lambda}_N^2}{2} M_N \right) M^2 + a s_1 M^2 \exp[-(s_1 - M_N^2)/M^2] \,\delta s_1 \,. \tag{23}$$

The corresponding sum rule from the $\frac{1}{4}$ structure [7–9] is unaffected by leading instanton corrections,

e

$$\frac{e^{M_N^2/M^2}}{6} \left[-aM^4 \,\delta m E_0 L^{-4/9} - \frac{4}{3}M^2 \,\gamma a^2 L^{4/9} + \frac{m_0^2}{6} \,\delta m M^2 a L^{-8/9} + \frac{m_0^2}{3} \,\gamma a^2 L^{-2/27} \right] \\ = \tilde{\lambda}_N^2 M_N \,\delta M_N - \frac{\delta \tilde{\lambda}_N^2}{2}M^2 + \frac{1}{4} \left(s_q^2 + \frac{b}{2} \right) M^2 \\ \times \exp[-(s_q - M_N^2)/M^2] L^{-4/9} \delta s_q \,. \tag{24}$$

The two parameters $b = \langle g_s^2 G_{\mu\nu}^a G_a^{\mu\nu} \rangle = 0.5$ GeV⁴ and $m_0^2 \equiv \langle g_s \overline{q} \sigma \cdot Gq \rangle / \langle \overline{q}q \rangle_0 = 0.8$ GeV² are fixed at their standard values and $E_0 \equiv 1 - e^{-s_q/M^2}$.

Above we have written both sum rules, Eqs. (23) and (24), in their most general form, which allows for independent values of the isosymmetric continuum thresholds s_1 and s_q . Below we will, however, follow the standard practice and set $s_1 = s_q \equiv s_0$.

At this point it might be useful to recall the main assumptions and approximations which went into the OPE of these sum rules and into the parametrization of their phenomenological sides. (For more details see [18,9].) The short-distance expansion is carried out up to operators of dimension 6 and the perturbative part of the Wilson coefficients is calculated to leading order in the strong coupling α_s . Less systematic uncertainties arise from the not precisely known values of the condensates and from the standard factorization of the four-quark condensates.

As is common practice in sum rule calculations, the Wilson coefficients are calculated without explicit infrared cutoff since at scales up to about 0.5-1 GeV nonperturbative contributions from the condensates strongly dominate over the perturbative ones. The explicit removal of the latter becomes, therefore, practically unnecessary [31]. For the same reason, the condensates (and the quark masses) depend in the above range rather weakly on the renormalization scale. Even without explicitly specifying the infrared regularization scheme of the Wilson coefficients, scale-dependent quantities are understood to be taken at a μ in the above range, and we use specifically $\mu=0.5$ GeV.

On the phenomenological side the main assumption is that of local duality between the hadron and quark-gluon descriptions of the continuum. It has been found to work well in many sum rule studies and also in recent lattice simulations of point-to-point correlators [26]. In our context it is put to a more difficult test since we consider differences of two spectral functions. Here even more than in the single nucleon sum rules the exponential Borel suppression of continuum contributions is important in order to increase the sensitivity of the sum rules to the ground state contributions.

In the numerical evaluation of the sum rules the upper limit of the Borel interval is determined such that contributions from the continuum do not exceed a given percentage of the full OPE contribution. Otherwise the sum rules would be relatively less sensitive to the pole contribution of interest and a good fit quality would become a trivial consequence of continuum domination (instead of being a consistency criterion), since the continuum is modeled after the leading OPE behavior. Moderate continuum contributions are, therefore, a necessary condition for reliable sum rules, and in the next section we will check how these contributions are affected by the instanton terms.

VI. QUANTITATIVE SUM RULE ANALYSIS

The quantitative analysis of isospin violation in the nucleon sum rules aims at determining the isospin-breaking parameters on the phenomenological side from the best fit to the "theoretical" left-hand side. Taking all the other parameters from the standard, isosymmetric nucleon sum rules or from experiment, it would still require a four-parameter fit to determine δM_N , $\delta \tilde{\lambda}_N^2$, δs_q , and δs_1 independently. Limitations in the parametrization of the spectral densities and approximations on the theoretical side would, however, make such a fit unstable both with and without instantons.

In order to reduce the number of fit parameters, one is thus led to either fix the only phenomenologically known one, δM_N , at its experimental value [9] or to make assumptions relating at least two of the remaining isospin-breaking parameters. The authors of Ref. [7], for example, assume $\delta s_q = \delta s_1$ in their analysis or, alternatively, neglect differences in the effective continuum of proton and neutron channels entirely, i.e., $\delta s_q = \delta s_1 = 0$. Since such assumptions lack theoretical foundation, the associated errors cannot be reliably estimated or controlled. We thus prefer to follow the approach of Ref. [9], taking $\delta M_N^{\text{nonelm}} = 2.05 \pm 0.30$ MeV as input from phenomenology. This value is derived from the experimental mass difference $\delta M_N^{\text{expt}} = 1.29$ MeV [32] by subtracting the electromagnetic contribution δM_N^{elm} $= -0.76 \pm 0.30$ MeV [33].

For the isoscalar nucleon mass and quark condensate we use the standard values $M_N=940$ MeV and $\langle \bar{q}q \rangle_0 = -(225 \text{ MeV})^3$. The residuum of the isosymmetric nucleon pole, $\tilde{\lambda}_N^2 = 1.8 \text{ GeV}^6$, and the isospin average of the continuum threshold, $s_0 = 2.2 \text{ GeV}^2$, are obtained from the instanton-corrected nucleon mass sum rules [5] in the same Borel window as the one used below.

The isospin-breaking parameters $\delta \lambda_N^2$, δs_1 , and δs_q are then calculated by minimizing the difference between the left- and right-hand sides of the sum rules (23) and (24) under the logarithmic measure δ of Ref. [6] in the Borel-mass region 0.8 GeV² $\leq M^2 \leq 1.4$ GeV².

We performed this minimization for various values of γ in the range $-1 \times 10^{-2} \le \gamma \le -2 \times 10^{-3}$ discussed in Sec. II. We find a better agreement between both sum rules towards larger (and more conventional) values of $|\gamma|$ in this interval,



FIG. 1. Best fit of the RHS (continuous line) of the sum rules to the the LHS of the Π_q (dotted line) and Π_1 (dashed line) sum rules.



FIG. 2. The neutron-proton mass difference as a function of the Borel mass from the optimized Π_q (continuous line) and Π_1 (dashed line) sum rules.

whereas the analogous study of [9], which neglects instanton contributions, prefers an unusually small value, $|\gamma|=2\times10^{-3}$. For $\gamma=-1\times10^{-2}$, in particular, our best fit between left-hand side (LHS) and right-hand side (RHS) results in the parameter values

$$\delta \tilde{\lambda}_N^2 = -2.1 \times 10^{-4} \text{ GeV}^6, \quad \delta s_1 = -1.7 \times 10^{-2} \text{ GeV}^2, \\ \delta s_q = 1.03 \times 10^{-3} \text{ GeV}^2.$$
(25)

Figures 1–3 show different aspects of this fit. In order to compare the fits of the optimized Π_q and Π_1 sum rules, we transfer all but the first two terms on the RHS of the Π_q sum rule (24) to the left and we rewrite the Π_1 sum rule (23) analogously, so that the same two terms, $\tilde{\lambda}_N^2 M_N \delta M_N - (\delta \tilde{\lambda}_N^2/2) M^2$, remain on its RHS. Figure 1 compares this RHS (continuous line) with the modified LHS of the Π_q (dotted line) and Π_1 (dashed line) sum rules.

In Fig. 2 we plot the resulting neutron-proton mass difference δM_N as a function of M^2 , obtained by solving both optimized sum rules for $\delta M_N(M^2)$. These curves show an extended stability plateau, which confirms the satisfactory agreement between the two sum rules. Indeed, this Borelmass independence of observables is the only intrinsic consistency criterion for the sum rules.

In order to compare the relative size and behavior of the OPE and instanton contributions to the Π_1 sum rule (23)



FIG. 3. Instanton and OPE contributions to the LHS of the Π_1 sum rule. Their sum (dashed line) is fitted to the RHS (continuous line).



FIG. 4. Same as Fig. 1 for the sum rules optimized without instanton contributions and with $\gamma = -2 \times 10^{-3}$.

(recall that the Π_q sum rule does not receive instanton corrections), we display both of them separately, as well as their sum and the fit to the optimized RHS of Eq. (23), in Fig. 3. The instanton terms reach almost the magnitude of the perturbative and power terms and play clearly an important role in determining the sum rule results. The usual practice to neglect these contributions seems thus unjustified.

It is also instructive to compare our results of Figs. 1 and 2 with the analogous curves, but calculated without instanton corrections. Recall that in this case the $\langle \overline{uu}d\overline{d} \rangle$ part of the four-quark condensate has to be restored in Eq. (23), which changes the factor 4/3 in its Wilson coefficient to -2/3. As already noted, a smaller absolute value of γ is favored in this case, and the curves in Figs. 4 and 5 were obtained by optimizing the sum rules with $\gamma = -2 \times 10^{-3}$. Up to small corrections from the neglected eight-dimensional condensates, they correspond to the ones⁶ analyzed in [9].

From Fig. 4 it is also clear that rather different values of the isospin-breaking parameters ($\delta \tilde{\lambda}_N^2 = 1.4 \times 10^{-2} \text{ GeV}^6$, $\delta s_q = 7.0 \times 10^{-3} \text{ GeV}^2$, $\delta s_1 = 1.2 \times 10^{-2} \text{ GeV}^2$) are required to fit phenomenological and theoretical sides as long as instanton contributions are neglected. The difference between the pole strength of neutron and proton, in particular, becomes about two orders of magnitude larger and changes sign.

More importantly, however, the small modulus of γ preferred by this fit has an unwelcome consequence. Closer inspection of the sum rules reveals that decreasing values of $|\gamma|$ lead to increasing contributions from the continuum relative to the power corrections in the optimized sum rules. Indeed, the parameter values used above correspond to a continuum contribution of 90% in the chirally odd sum rule (and about 37% in the chirally even sum rule). This continuum domination casts serious doubts on the reliability of the chirally odd sum rule, even if fit quality and stability seem satisfactory (cf. Fig. 5). In both instanton-corrected sum rules, on the other hand, the continuum contributions remain moderate (about 20%).

⁶The sum rule of Ref. [9] contains an error in the coefficient of the four-quark condensate which we have corrected.



FIG. 5. Same as Fig. 2 for the sum rules optimized without instanton contributions and with $\gamma = -2 \times 10^{-3}$.

It is interesting to note that another recent sum rule analysis of γ [34], which is based on the mass splitting in the *D* and *D** isospin dublets, also finds a small value $|\gamma| \sim 2.5 \times 10^{-3}$, which is close to the result of Ref. [9]. Since it is derived from an independent sum rule the discrepancy with the result of chiral perturbation theory might have a different origin in the *D* meson channel. This issue and the role of instanton corrections in this channel deserve further investigation, which will be the subject of a forthcoming publication [35].

VII. SUMMARY AND CONCLUSIONS

In this paper we study the role of instantons in the dynamics of isospin violation, as it manifests itself in the shortdistance expansion of the nucleon correlation functions. Isospin-breaking effects lead to differences between the neutron and proton correlators, which can be translated via dispersion relations into isopin-violating vacuum and nucleon parameters.

The isospin-breaking instanton corrections to the nucleon correlators show several characteristic qualitative features. As a consequence of using Ioffe's interpolating field, instanton contributions are absent in the chirally even amplitudes. Moreover, the difference of these amplitudes for neutron and proton is not affected by instanton corrections for any choice of the interpolating field.

The chirally odd amplitude, on the other hand, receives instanton contributions of almost the magnitude of the standard OPE terms, as in the isosymmetric case. They correct the Wilson coefficients of the unit operator and of the quark condensates. The difference between the neutron and proton amplitudes is, in fact, mainly generated by the quark condensate terms, i.e., by isopin-violating quark modes in the vacuum.

This confirms the general expectation that isospinbreaking effects in hadrons are physically subtle not only because they are small, but in particular because they depend sensitively on non-valence-quark physics. This is a challenging and little-tested regime for hadron models, which often neglect vacuum effects altogether and thus miss important sources of isospin asymmetry. Bag (and other quark) model calculations which evaluate instanton-induced quark interactions between SU(6) states with good isospin fail, for example, to find instanton contributions to the neutron-proton mass difference. The instanton-corrected OPE, on the other hand, contains vacuum physics at short distances and thus provides a more reliable and model-independent basis for the study of isospin-breaking effects.

The link between the correlators and nucleon properties is established by dispersion relations and takes the form of two QCD sum rules for the difference of the neutron and proton amplitudes. In adopting an approach for their quantitative analysis one has to decide between several alternatives. Taking the RHS to be the difference of the conventional polecontinuum *Ansätze* for the neutron and proton, it contains four isospin-breaking parameters which cannot be determined independently from a stable fit, even if instanton corrections are taken into account. In this situation one can either assume relations between these parameters or one can fix the only phenomenologically known one, the nucleon mass difference, at its experimental value. We adopt the latter approach since it does not introduce additional assumptions with uncontrolled theoretical errors.

The resulting sum rules, including the instanton corrections, are stable and receive only moderate (~20%) continuum contributions. This is a clear improvement over the analogous analysis without the instanton terms, where the continuum dominates. At the same time, the instanton contributions reduce the difference between the nucleon pole strengths and enhance the corresponding shift in the effective continuum thresholds. Moreover, and perhaps most importantly, the optimization of the sum rules with direct instanton effects favors larger and more standard values for the modulus of the isovector quark condensate, $|\gamma| \approx 10^{-2}$, which are close to those found in the chiral analysis.

We also tested an alternative approach towards the sum rule analysis. In this case the differences between proton and neutron continuum thresholds in both sum rules were assumed to be equal and the neutron-proton mass difference δM_N was determined from the fit. Inclusion of the instanton part allows a consistent fit of both sum rules, which seems otherwise impossible. The value of δM_N is then, however, overestimated by about 80%. This puts the initial assumption of an equal deviation of neutron and proton thresholds from the isoscalar position into question. It also supports our preference for the analysis method discussed above, which does not require *ad hoc* assumptions to relate fit parameters.

We conclude that instanton corrections play a significant role in the analysis of isospin breaking in nucleon sum rules. They, for example, strongly affect the results for the difference between the nucleon pole strengths and for the shifts in the effective continuum thresholds. In addition, the instanton corrections enhance the internal consistency of the sum rules and predict a larger and more standard value for the modulus of the quark condensate difference, $|\gamma| \approx (0.8-1) \times 10^{-2}$.

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