New chiral-symmetry-breaking operators in 
pseudoscalar QCD sum rules

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Abstract

Nonperturbative Wilson coefficients associated with the leading chiral-symmetry-breaking operators in the operator product expansion of the pseudoscalar QCD correlation function are derived. Implementation of the new, instanton-induced operators enables the corresponding spectral sum rule to reproduce the small pion mass scale, thereby reconciling it with Goldstone’s theorem. The same operators suppress the contributions of pionic resonances. Several predictions and structural insights from the new sum rule are discussed.
The arguably most characteristic pion property is its mass well below all other hadronic mass scales. This special feature has long been understood as a consequence of spontaneous chiral symmetry breaking (SCSB) in the QCD vacuum \[1\], which renders the pion a (quasi-) Goldstone boson and manifests itself in the finite vacuum expectation values of chirality-changing operators like the quark condensate \(\langle \bar{q}q \rangle\). One would therefore expect the QCD sum-rule approach \[2\], which explicitly links hadron properties by means of the operator product expansion (OPE) to such condensates, to provide a privileged source of information on the Goldstone nature of the pion and, in particular, to predict its small mass scale as a consequence of chiral-symmetry-breaking (CSB) condensates.

Surprisingly, this expectation is not borne out by the existing analyses of the pseudoscalar sum rule. They fail to predict a pion mass below standard hadronic scales \[2\], and the contributions from chirality-changing condensates are too strongly suppressed (by factors of the light quark masses) to have a notable impact on the resulting pion properties. This confronts us with a fundamental puzzle which threatens to unsettle the conceptual basis of the QCD-sum-rule approach: why is the conventional OPE of the pseudoscalar correlator practically blind to spontaneous chiral symmetry breaking, i.e. to exactly that element of QCD vacuum physics which profoundly affects the Goldstone boson channel?

Additional contributions - neglected in the standard OPE but potentially enhanced in the pseudoscalar channel - could provide an attractive resolution of this puzzle. One such contribution, a low-dimensional power correction conjectured to originate from ultraviolet-sensitive physics, has been proposed in \[3\]. Besides probably being small \[4\], however, this term is chirally invariant and therefore unlikely to significantly improve the pion mass prediction. Hard (so-called direct) instanton corrections to the unit-operator coefficient \[5–7\], although of substantial size, also proved unable to generate the physical pion mass scale \[8\]. The reason is probably the same as above: these contributions are chirally invariant (as their perturbative counterparts) and multiply the likewise chirally invariant unit operator.

The above examples illustrate that information related to SCSB can enter the OPE only through chiral-symmetry-breaking condensates (since it originates from soft vacuum
physics. In search for missing physics related to such condensates, we will identify and calculate in this letter the leading nonperturbative corrections to the Wilson coefficients associated with the lowest-dimensional CSB operators. These new contributions arise from small instantons and have the potential to resolve the above-mentioned puzzle since instantons couple particularly strongly to pseudoscalar interpolating fields [5,6] and generate Wilson coefficients which are not suppressed by light-quark mass factors (in contrast to their perturbative counterparts).

We start from the π⁰ correlation function

\[ \Pi(x) = \langle 0 | T j_{\pi^0}(x) j_{\pi^0}(0) | 0 \rangle, \]  

based on the pseudoscalar interpolator

\[ j_{\pi^0} = \sqrt{\frac{1}{2}} (\bar{u} i \gamma_5 u - \bar{d} i \gamma_5 d), \]  

which has an instanton-improved OPE (IOPE) (for a review see [9]) of the general form

\[ \Pi^{(IOPE)}(Q^2) = i \int d^4 x e^{iqx} \langle 0 | T j_{\pi^0}(x) j_{\pi^0}(0) | 0 \rangle^{(IOPE)} = \sum_n C_{\hat{O}_n}(Q^2; \mu) \langle \hat{O}_n(\mu) \rangle \]  

\( (Q^2 = -q^2 \geq 1 \text{ GeV}, \mu \lesssim 1 \text{ GeV is the operator renomalization scale}).\)

The perturbative parts \( C_{\hat{O}_n}^{(pert)} \) of the Wilson coefficients, to \( O(\alpha_s) \) for the unit operator and to leading order for all remaining operators up to mass dimension \( d = 6 \), are [2,10]

\[ C_{\hat{O}_1}^{(pert)}(Q^2; \mu) = \frac{3}{8 \pi^2} Q^2 \ln \frac{Q^2}{\mu^2} \left[ 1 + \frac{17}{3} \frac{\alpha_s}{\pi} - \frac{\alpha_s}{\pi} \ln \frac{Q^2}{\mu^2} \right], \]  

\[ C_{\hat{O}_{\bar{q} q}}^{(pert)}(Q^2) = -\frac{m_q}{Q^2}, \quad C_{\hat{O}_4}^{(pert)}(Q^2) = \frac{1}{8 \pi Q^2}, \]  

\[ C_{\hat{O}_5}^{(pert)}(Q^2) = -C_{\hat{O}_6}^{(pert)}(Q^2) = -\frac{\pi}{Q^2}, \]  

where \( \hat{O}_{4,5} \) are the four-quark operators

\[ \hat{O}_4 = -\alpha (\bar{u} \sigma_{\mu \nu} t^a u) (\bar{d} \sigma_{\mu \nu} t^a d), \]  

\[ \hat{O}_5 = \frac{1}{2} \alpha \left[ (\bar{u} \sigma_{\mu \nu} t^a u)^2 + (\bar{d} \sigma_{\mu \nu} t^a d)^2 \right] + \frac{1}{3} \alpha (\bar{u} \gamma_{\mu} t^a u + \bar{d} \gamma_{\mu} t^a d) \left( \sum_{u,d,s} \bar{q}_\gamma \gamma_{\mu} t^a q \right) \]
\( t^a = \lambda^a / 2 \), where \( \lambda^a \) are the Gell-Mann matrices).

Each term in the IOPE (3) factorizes into contributions from hard modes with momenta \( |k| > \mu \), contained in the \( C_{\hat{O_n}} \), and from soft modes with \( |k| \leq \mu \) in the operators \( \hat{O}_n \).

Despite widespread belief (based on asymptotic freedom) there are hadron channels where this does not even approximately amount to a factorization of perturbative and nonperturbative physics (at \( \mu \sim 1 \text{ GeV} \)). Indeed, early conjectures \[6\] and substantial recent evidence \[1\] corroborate that (semi-) hard nonperturbative contributions due to small instantons are quantitatively relevant or even dominant in several hadronic correlators.

The pseudoscalar correlator, in particular, is known to receive exceptionally strong direct-instanton contributions to the unit-operator coefficient,

\[
C^{(I+\bar{I})}_1 (Q^2) = \int d\rho \rho \frac{\bar{m}_{q,2}^2(\rho) + \bar{m}_{d,2}^2(\rho)}{\bar{m}_{u,2}^2(\rho)} (Q\rho)^2 K_1^2 (Q\rho) \tag{9}
\]

\((I, \ (\bar{I}))\) refers to the (anti-) instanton closest to \(x\), \(n(\rho)\) is the vacuum distribution of instantons with size \(\rho\), and \(K_1(z)\) is a McDonald function \[12\], which arise from the propagation of both quark and antiquark (ejected by (2)) in the zero mode of the instanton field \[1\] and can be obtained by means of semiclassical techniques \[6,9\]. Due to interactions with ambient, long-wavelength vacuum fields (including other instantons) \[14\] the quarks acquire an effective mass \(\bar{m}_{q,2}(\rho)\) (the index indicates that two quarks are propagating in zero modes). The quantitative sum-rule analysis below only requires the value of \(\bar{m}_{q,2}\) at the average instanton size \(\bar{\rho} \simeq 0.33 \text{ fm}\) for which we adopt the recent estimate \(\bar{m}_{q,2}(\bar{\rho}) \equiv \bar{m}_{q,2} \simeq 85 \text{ MeV}\) obtained from instanton-liquid model (ILM) simulations of the pseudoscalar correlator \[15\]. The \(\bar{m}_{q,2}\)-dependence of the results will be discussed in \[10\].

All so far considered contributions to the IOPE coefficients are either associated with chirally-invariant operators or too strongly suppressed (note the factor \(m_q\) in \(C^{(\text{pert})}_{\bar{q}q}\)) to generate more than minute corrections to the pion mass. Hence at this stage - which

\[^1C^{(I+\bar{I})}_1 (Q^2)\] has the same momentum dependence as several instanton contributions (which arise from the analogous diquark loop) to baryon sum rules \[11,13\].
represents the current state of the art - the IOPE does contain virtually no information on the soft vacuum fields which are responsible for the spontaneous breakdown of chiral symmetry. Therefore it is not surprising that the corresponding sum rule is unable to generate the low mass scale which characterizes the Goldstone pion [8].

As we have argued above, there are reasons to believe that the missing information on SCSB is activated by nonperturbative contributions to the Wilson coefficients of chirally noninvariant operators which so far went unnoticed. Furthermore, direct instantons are promising candidates for such contributions since (i) they provide the leading nonperturbative deviations from asymptotic freedom, (ii) they are likely to play an important rôle in the dynamics of SCSB and in the strong flavor-mixing among pseudoscalar mesons [3], (iii) their small average size $\bar{\rho} \lesssim \mu^{-1}$ allows them to contribute strongly to the Wilson coefficients, (iv) light-quark-mass suppression factors are absent, (v) the sensitivity of spin-0 meson channels to instanton-induced short-distance physics is enhanced [4-7], and finally (vi) recent lattice measurements find the pseudoscalar correlator dominated by contributions from instanton-induced quark (quasi-) zero modes [9].

We are thus led to derive the instanton contributions to the Wilson coefficients associated with the dominant (i.e. lowest-dimensional) chiral-symmetry-breaking operators of the IOPE, $\bar{q}q$ and $g\bar{q}\sigma Gq$. They can be calculated as the leading terms in the semiclassical expansion of the correlator around the (anti-) instanton in the background of long-wavelength quark and gluon vacuum fields. We postpone a detailed description of this calculation to [16] and present here just the results,

$$C_{\bar{q}q}^{(1+1)} (Q^2) = -\frac{\pi^2}{2} \int d\rho n(\rho) \frac{\rho^4}{m_{q,1}(\rho)} \times \int_0^\infty d\alpha \frac{d\alpha}{\alpha^2} \frac{1}{\Gamma(5/2; 3; -1/4\alpha)} \int_0^\infty d\beta \frac{1}{\Gamma(3/2; 2; -1/4\beta)} e^{-(\alpha+\beta)Q^2\rho^2}$$

where $1F_1 (a; b; z)$ is the confluent hypergeometric function [12]) for the quark condensate coefficient and

$2$The same holds for spin-0 glueballs [18].
for the coefficient associated with the mixed quark-gluon operator \( g_s \bar{q} \sigma G q \). This operator appears for the first time in the OPE of the pseudoscalar correlator. As expected, the above coefficients are not suppressed by small quark masses and can be several orders of magnitude larger than their perturbative counterparts. Since they arise from only one quark propagating in the zero-mode state (while the other, soft one contributes to the accompanying operator) we have denoted the corresponding effective mass \( \bar{m}_{q,1}(\rho) \).

Note that \( \bar{m}_{q,1} \) does not equal \( \bar{m}_{q,2} \) although both emerge from a mean-field picture of quark interactions with soft vacuum fields. The first main difference between the two is rooted in the fact that they arise from averages over the ensemble of vacuum fields (approximated, e.g., by instantons in the ILM). Due to the fluctuations in this ensemble one should not expect averages over more than one zero-mode propagator to factorize into separate averages over each propagator, and as a consequence \( \bar{m}_{q,1} \neq \bar{m}_{q,2} \). This can be verified explicitly in the ILM framework \[15\].

The second difference is specific to the IOPE: while in the two-zero-mode contribution (9) the external momentum \( Q \) is shared between both quark lines, the full (i.e. maximal) \( Q \) flows through the one zero-mode quark line in (10) and (11). Now, in more complete treatments of the interactions with the vacuum background fields the effective masses will become momentum-dependent quark self-energies \( \bar{m}_q(k) \). For momenta much larger than the chiral symmetry breaking scale, \( k \gg \Lambda_{CSB} \), these self-energies become insensitive to the soft CSB vacuum modes and approach the current quark mass, \( \bar{m}_q(k \to \infty) \to m_q \). Since the effective mean-field masses can be considered as momentum averages of such quark self-energies (or \( \bar{m}_{q,i} = \bar{m}_q(\bar{Q}_i) \) with \( \bar{Q}_i \) the typical momentum scale), one expects a scale hierarchy

\[
\bar{m}_q(Q = 0) \geq \bar{m}_{q,2} \geq \bar{m}_{q,1} \geq m_q
\]  

(12)
for all $\rho$. In order to get an idea of the size of $\bar{m}_{q,1} = \bar{m}_{q,1} (\bar{\rho}, \bar{Q}_1)$, we will adopt the value of the quark self-energy $M (k)$ in the large-$N_c$ approximation to the ILM \cite{20} at the momentum transfer $\bar{Q}_1 = 1.5 \text{ GeV}$ (the mean value of the interval $Q \in [1, 2] \text{ GeV}$ relevant for the sum rule below).

$$\bar{m}_{q,1} \sim M (\bar{Q} = 1.5 \text{ GeV}) = \frac{M (0) \bar{Q}^2}{4\pi^2 \bar{\rho}^2} \varphi^2 (\bar{Q}) \approx 20 \text{ MeV},$$ \hspace{1cm} (13)

where $M (0) \approx 0.3 \text{ GeV}$ and $\varphi (k)$ is a combination of modified Bessel functions given in \cite{20}. Since $\bar{m}_{q,1} \approx 0.02 \text{ GeV}$ is rather close to the lower end of the admissible region \cite{12}, the size of the instanton-induced coefficients (II) and (I) will reach about one half of their upper bound. The impact of different choices for $\bar{m}_{q,1}$ on predictions and stability of the sum rule will be discussed in \cite{16}.

Having calculated the IOPE of the pseudoscalar correlator up to $d = 6$, we now turn to the associated QCD sum rule. It will be convenient to rewrite the different parts $\Pi^{(X)} (Q^2) \ (X \in \{ \text{pert}, I + \bar{I}, \ldots \})$ of the correlator by means of the dispersion relation as

$$\Pi^{(X)} (\tau) \equiv \hat{B}_\tau \Pi^{(X)} (Q^2) = \frac{1}{\pi} \hat{B}_\tau \int ds \frac{\text{Im} \Pi^{(X)} (-s)}{s + Q^2} = \frac{1}{\pi} \int ds \text{Im} \Pi^{(X)} (-s) e^{-s\tau}. \hspace{1cm} (14)$$

In Eq. (14) we have already applied the obligatoy Borel transform $\hat{B}_\tau$ which improves IOPE convergence, removes subtraction terms and emphasizes the ground-state contribution to the correlator \cite{2}.

A spectral sum rule is then obtained by equating the IOPE description $\Pi^{(IOPE)} (\tau)$ of the correlator (in the $\tau$ region where it is reliable, see below) to a standard hadronic representation $\Pi^{(phen)} (\tau)$ whose spectral function consists of pole and duality-continuum parts:

$$\text{Im} \Pi^{(phen)} (-s; s_0) = \text{Im} \Pi^{(pole)} (-s) + \text{Im} \Pi^{(cont)} (-s; s_0). \hspace{1cm} (15)$$

$^3$The analogous estimate for $\bar{m}_{q,2}$ yields the value $\bar{m}_{q,2} \approx 85 \text{ MeV}$ of Ref. \cite{15} at $\bar{Q}_2/\Lambda_{CSB} \approx 0.85$, which might explain why $\bar{m}_{q,2}$ is significantly smaller than typical constituent quark masses.
The effective threshold $s_0$ delimits the duality interval of the continuum into which we include, besides the standard OPE part, the instanton contributions:

$$\text{Im} \Pi^{(\text{cont})}(-s; s_0) = \left[ \text{Im} \Pi^{(\text{OPE})}(-s) + \text{Im} \Pi^{(I+I)}(-s) \right] \theta(s - s_0). \quad (16)$$

The instanton part will play an important rôle in the ensuing sum-rule analysis. In the pole (i.e. resonance) contribution we allow, besides the pion, also for its first excitation $\pi'$,

$$\text{Im} \Pi^{(\text{pole})}(s) = \pi \lambda^{2}_{\pi} \delta(s - m^{2}_{\pi}) + \pi \lambda^{2}_{\pi'} \delta(s - m^{2}_{\pi'}), \quad (17)$$

where $m_{\pi}$ and $m_{\pi'}$ are the masses of the pion and the $\pi'$, and $\lambda_{\pi} = \sqrt{2} f_{\pi} K \left( f^{(\text{exp})}_{\pi} = 93 \text{ MeV} \right)$ with $K = m^{2}_{\pi} / (m_{u} + m_{d})$. Including the $\pi'$ resonance explicitly enables us to predict its strength $\lambda^{2}_{\pi'}$ from the sum-rule analysis. Thus we can directly determine the quantitative impact of the $\pi'$ and decide whether it dominates the $\pi$ contribution (as suggested in [8]) or whether it can be absorbed into the duality continuum (as in other QCD sum-rules).

Subtracting the continuum contributions of Eq. (16) from the IOPE, separately for each operator $\hat{O}_{n}$, we can write the sum rule as

$$\mathcal{R}(\tau; s_0) \equiv \Pi^{(\text{IOPE})}(\tau) - \Pi^{(\text{cont})}(\tau; s_0)$$

$$= \sum_{n} \left[ \mathcal{R}^{(\text{pert})}_{\hat{O}_{n}}(\tau; s_0) + \mathcal{R}^{(I+I)}_{\hat{O}_{n}}(\tau; s_0) \right] = \lambda^{2}_{\pi} e^{-m^{2}_{\pi} \tau} + \lambda^{2}_{\pi'} e^{-m^{2}_{\pi'} \tau}, \quad (18)$$

where the pole contributions are isolated on the right-hand-side and where we have defined

$$\mathcal{R}^{(X)}_{\hat{O}_{n}}(\tau; s_0) \equiv \Pi^{(X)}_{\hat{O}_{n}}(\tau) - \frac{1}{\pi} \int_{0}^{\infty} ds \text{Im} \Pi^{(X)}_{\hat{O}_{n}}(-s) \theta(s - s_0) e^{-\tau s}$$

$$= \frac{1}{\pi} \int_{0}^{s_0} ds \langle \hat{O}_{n} \rangle \text{Im} C^{(X)}_{\hat{O}_{n}}(-s) e^{-\tau s}. \quad (19)$$

It remains to calculate the imaginary parts of the Wilson coefficients in the timelike region from the explicit expressions for the $C^{(X)}_{\hat{O}}$ given above. For the perturbative Wilson coefficients we find

$$\text{Im} C^{(\text{pert})}_{1}(-s) = \frac{3}{8 \pi} s \left\{ 1 + \frac{\alpha_{s}}{\pi} \left[ \frac{17}{3} - 2 \ln \left( \frac{s}{\mu^{2}} \right) \right] \right\}, \quad (20)$$

$$\text{Im} C^{(\text{pert})}_{\bar{q}q}(-s) = -\pi m_{q} \delta(s), \quad \text{Im} C^{(\text{pert})}_{\alpha G^{2}}(-s) = \frac{1}{8} \delta(s), \quad (21)$$

$$\text{Im} C^{(\text{pert})}_{1}(-s) = -\text{Im} C^{(\text{pert})}_{2}(-s) = \pi^{2} \delta'(s). \quad (22)$$
The instanton-induced contributions can be obtained in closed form from the imaginary parts of the coefficients (9), (10) and (11). The unit-operator coefficient (9) gives

\[ \text{Im} C_{1}^{(1+I)} (-s) = -\frac{\pi^2}{2} \int d\rho n(\rho) \rho^2 \frac{m_{u,2}^2(\rho) + m_{d,2}^2(\rho)}{m_{u,2}^2(\rho) m_{d,2}^2(\rho)} s J_1 (\sqrt{s}\rho) Y_1 (\sqrt{s}\rho). \]  (23)

The imaginary parts of the coefficients associated with chiral-symmetry-breaking operators have a more complex structure. They can be expressed in terms of the integrals

\[ I_{J_{i,j}} (s) = \int_0^1 d\eta \frac{\eta^{j+3} J_{i} (\sqrt{s}\rho\eta)}{\sqrt{1 - \eta^2}}, \quad I_{Y_{i,j}} (s) = \int_0^1 d\eta \frac{\eta^{j+3} Y_{i} (\sqrt{s}\rho\eta)}{\sqrt{1 - \eta^2}}, \]  (24)

where \( J_{i} (z) \) and \( Y_{i} (z) \) are Bessel and Neumann functions [12]. For the instanton contribution to the quark-condensate coefficient (10) we find

\[ \text{Im} C_{\bar{q}q}^{(1+I)} (-s) = -\frac{2^6\pi^2}{3} \int d\rho \frac{n(\rho) \rho^4}{m_{q,1}^2(\rho)} I_{J_{1,0}} (s) I_{Y_{1,0}} (s) - \frac{2^3\pi^3}{3} \int d\rho \frac{n(\rho) \rho^2}{m_{q,1}^2(\rho)} \delta (s) \]  (25)

and for the mixed condensate coefficient (11)

\[ \text{Im} C_{g\bar{q}Gq}^{(1+I)} (-s) = \frac{2^2\pi^2}{3} \int d\rho \frac{n(\rho) \rho^6}{m_{q,1}^2(\rho)} [2 I_{J_{0,1}} (s) I_{Y_{0,1}} (s) - I_{J_{1,2}} (s) I_{Y_{1,0}} (s) - I_{J_{1,0}} (s) I_{Y_{1,2}} (s)] - \frac{\pi^3}{2^2} \int d\rho \frac{n(\rho) \rho^4}{m_{q,1}^2(\rho)} \delta (s). \]  (26)

Note that both (25) and (26) receive strong contributions from \( s = 0 \) which significantly reduce the \( s_0 \)-dependence of the CSB terms \( R_{\bar{q}q} (\tau; s_0) \) and \( R_{g\bar{q}Gq} (\tau; s_0) \) (cf. Fig. 1b below).

For the quantitative analysis of the sum rule (18) we fix the IOPE parameters at standard values: \( \Lambda_{QCD} = 0.2 \text{ GeV} \), \( \langle \bar{q}q \rangle = -0.0156 \text{ GeV}^2 \), \( \langle \alpha_s G^2 \rangle = 0.04 \text{ GeV}^4 \), \( \langle g_{\bar{q}q} G q \rangle = m_0^2 \langle \bar{q}q \rangle \), \( m_0^2 = 0.8 \text{ GeV}^2 \), \( \langle \dot{O}_4 + \dot{O}_5 \rangle = (56\pi\alpha_s/27) \langle \bar{q}q \rangle^2 \). As in previous IOPE sum rules, we approximate the instanton distribution as \( n(\rho) = n\delta (\rho - \bar{\rho}) \) with \( n = 0.5 \text{ fm}^{-4} \) and \( \bar{\rho} = 0.33 \text{ fm} \). The standard RG improvement, finally, amounts to scaling \( \langle \dot{O}_n \rangle \rightarrow \xi^{2 - \gamma_n} \langle \dot{O}_n \rangle \) with \( \gamma_{1,\alpha_s G^2} = 0 \), \( \gamma_{\bar{q}q} = 1 \), \( \gamma_{g_{\bar{q}q} G q} = -1/6 \) and

\[ \xi (\tau) = -\frac{1}{2} \ln (\tau\Lambda^2)^{-4/9} \left[ 1 - \frac{290}{729} \frac{1}{\ln (\tau\Lambda^2)} + \frac{256}{729} \frac{\ln [-\ln (\tau\Lambda^2)]}{\ln (\tau\Lambda^2)} \right]. \]  (27)

\(^4\)Phenomenological, ILM and lattice evidence for these scales is discussed in [17].
to replacing $\alpha_s$ by the (two-loop) running coupling, and to substituting $\mu^2 \rightarrow 1/\tau$.

The resulting $\tau$- and $s_0$-dependence of $\mathcal{R}(\tau; s_0)$ is plotted in Fig. 1a. Note that for $\tau \gtrsim 1.4 \text{ GeV}^{-2}$ and $s_0 \gtrsim 2.5 \text{ GeV}^2$, $\mathcal{R}(\tau; s_0)$ becomes practically $s_0$-independent. This is a consequence of the exponential $\exp(-s\tau)$ in the integrands of (14) which renders the dispersive integrals insensitive to their upper integration limit $s_0$ whenever $\exp(-s_0\tau) \lesssim 10^{-2}$. Therefore, $s_0$ cannot be determined by the sum rule in this $(\tau, s_0)$-region. Another conspicuous feature of $\mathcal{R}(\tau; s_0)$ is the valley at intermediate $s_0$ and small $\tau$, which can be traced to the instanton continuum contribution of the unit-operator coefficient. In this $(\tau, s_0)$-region the sum rule does not match since the positive slopes in $\tau$-direction do not fit the decaying exponentials of the pole contributions. In the $s_0$-region around 2 GeV$^2$ (i.e. around the values which one would expect from duality arguments), however, $\mathcal{R}(\tau; s_0)$ shows an extended “mountain ridge” with the slow decay in $\tau$ which matches an exponential containing a rather small mass. Thus we have qualitatively identified the area in which the sum rule will optimize, and we have found that the pion contribution must be sizeable. Both observations will be confirmed by the quantitative analysis below.

Figure 1b exhibits the $\tau$- and $s_0$-dependence of the new, instanton-induced CSB contributions to $\mathcal{R}(\tau; s_0)$, i.e. of

$$\mathcal{R}^{(CSB)}(\tau; s_0) \equiv \mathcal{R}_{qq}^{(I+\bar{I})}(\tau; s_0) + \mathcal{R}_{qgGq}^{(I+\bar{I})}(\tau; s_0). \quad (28)$$

The essential message of this plot is that in the physically meaningful $(\tau, s_0)$-region where $s_0 \leq 4 \text{ GeV}^2$ or $\tau \geq 0.4 \text{ GeV}^{-2}$, the CSB contributions are monotonically increasing with $\tau$. In fact, those are the only relevant contributions to the IOPE whose slope is positive. Moreover, the slope at small $\tau$ becomes maximal in the $s_0$-region around 2 GeV$^2$ where the sum rule optimally matches. Thus these CSB contributions overcome much of the negative slope originating from the chirally invariant operators (with both perturbative and instanton-induced coefficients) and thereby lower the prediction for the pion mass. This qualitative result demonstrates how the CSB condensates, “activated” by direct instantons, can reconcile the pseudoscalar sum rule with Goldstone’s theorem. As a byproduct, they
enhance the strength of the pion contributions relative to those from higher resonances.

The main task of the quantitative sum-rule analysis is to find those values of the hadronic parameters to be determined for which both sides of (15) optimally match in the fiducial \( \tau \)-region. The latter is obtained from the standard requirements that (i) the highest-dimensional operators should contribute less than 10% to \( \mathcal{R}(\tau; s_0) \), that (ii) multi-instanton effects should be negligible, and that (iii) the continuum contributions should be limited to maximally 50% of the total \( \mathcal{R}(\tau; s_0) \). Since one sum rule cannot reliably determine all five hadronic parameters, we have chosen to fix those best known from experiment, \( m_{\pi^0} = 135 \) MeV and \( m_{\pi'} = 1300 \) MeV [22], and to determine the values of the remaining ones\(^5\) i.e. \( s_0 \), \( \lambda_\pi \) and \( \lambda_{\pi'} \). Both sides of the optimized sum rule are shown in Fig. 2. Their good match confirms the consistency and stability of the sum rule. The resulting values for the couplings are \( \lambda_\pi^2 = 0.078 \) GeV\(^4\) and \( \lambda_{\pi'}^2 = 0.032 \) GeV\(^4\), while the continuum threshold becomes \( s_0 = 1.84 \) GeV\(^2\). With \( f_\pi = 93 \) MeV and \( m_\pi = 135 \) MeV this implies \( m_u + m_d = \sqrt{2} f_\pi m_\pi^2/\lambda_\pi \simeq 9.0 \) MeV (at \( \mu \sim 1 \) GeV), within the estimated range \((6.75 - 16.2 \) MeV\) of Ref. [22].

Fig. 2 also shows the individual contributions \( \mathcal{R}_{1+\alpha G^2+O_4+O_5}^{(pert)} \), \( \mathcal{R}_1^{(I+I)} \), \( \mathcal{R}_{qq}^{(I+I)} \), and \( \mathcal{R}_{g\bar{q}Gqq}^{(I+I)} \) to the left-hand side of the sum rule. The instanton contributions can be seen to dominate, and the positive slope of the CSB parts indeed compensates most of the negative slope brought in by the chirally invariant ones. As expected, \( \mathcal{R}_1^{(I+I)} \) contributes with (strongly) negative slope. This explains why the sum rule of Ref. [8], which took exclusively this direct-instanton contribution (without it’s continuum part) into account, could not be stabilized without a strong resonance in the 1 GeV region.

Implementing the CSB operators (and their continuum contributions) increases the relative strength of the pion pole to \( (\lambda_\pi^2/\lambda_{\pi'}^2) \exp(m_{\pi'} - m_\pi) \simeq 8 - 70 \) in the fiducial Borel

\(^5\)Alternative analysis strategies will be considered in [16]. We have checked, in particular, that the sum rule predicts the small pion mass scale, \( m_\pi \simeq 140 \) MeV, if \( \lambda_\pi \) is fixed at it’s average phenomenological value \( \lambda_\pi \simeq 0.27 \) GeV\(^2\).
domain. As a consequence, the pion dominates while the \( \pi' \) contributions become negligible. In conjunction with the relatively small value of the continuum threshold \( s_0 = 1.84 \text{ GeV}^2 \) this suggests that the excited-state contributions can be absorbed into the duality continuum (as in practically all other sum-rule channels). The pion dominance seems natural in view of the exceptionally large mass difference between ground state and first excitation in the pseudoscalar channel. Moreover, it is consistent with lattice simulations of mesonic point-to-point correlators which find the pseudoscalar correlator well described by just the ground state pole and the duality continuum \[23\].

In summary, we have introduced instanton-generated Wilson coefficients associated with the leading chiral-symmetry-breaking operators in the IOPE of the pseudoscalar correlator. The new contributions are fully nonperturbative (both at soft and hard momenta) and supply previously missing information about spontaneous chiral symmetry breaking which reconciles the associated pseudoscalar sum rule with Goldstone's theorem. As a consequence, this sum rule becomes the first in its channel which is able to reproduce the light mass scale of the pion. This resolves the puzzle stated in the introduction. Moreover, the chirally-odd operators suppress the contributions from higher-lying resonances, which can therefore be subsumed into the dispersive continuum. Both effects, as well as the stability of the sum rule, are enhanced by the instanton-induced continuum contributions. Additional implications of the new operators, e.g. for the calculation of the light quark mass values on the basis of pseudoscalar sum rules, will be discussed elsewhere \[16\].
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I. FIGURE CAPTIONS

1. Fig. 1a: The theoretical side of the sum rule, $R(\tau; s_0)$, with $\bar{m}_{q,1} = 20$ MeV and $\bar{m}_{q,2} = 85$ MeV.

2. Fig. 1b: The instanton-induced contributions of the chiral-symmetry-breaking operators, $R^{(CSB)}(\tau; s_0) \equiv R^{(I+\bar{I})}_{\bar{q}q}(\tau; s_0) + R^{(I+\bar{I})}_{\bar{q}q G \sigma q}(\tau; s_0)$, to the theoretical side of the sum rule.

3. Fig. 2: The right-hand-side (full line) of the optimized sum rule is compared to the theoretical side $R(\tau; s_0 = 1.84 \text{ GeV})$ (dotted). The contributions to $R$ from the perturbative ($R^{(\text{pert})}$, short-dashed) and instanton-induced ($R^{(I+\bar{I})}_{\bar{q}q}$ dot-dashed, $R^{(I+\bar{I})}_{\bar{q}q G \sigma q}$ dot-dot-dashed, their sum dashed) Wilson coefficients are also plotted separately.
\[ R^{(X)}(\tau; S_0) \]

\( \tau \) (GeV\(^{-2}\))
$R^{(CSB)}(\tau; s_0)$

$\tau$ (GeV$^{-2}$)

$s_0$ (GeV$^2$)
$R(\tau; s_0)$ vs. $s_0$ (GeV$^2$) and $\tau$ (GeV$^{-2}$)