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Constraint on the light quark mass m_q from QCD sum rules in the $I=0$ scalar channel

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In this paper, we reanalyze the $I=0$ scalar channel with the improved Monte-Carlo-based QCD sum rules, which combines the rigorous Hölder-inequality-determined sum rule window and a parametrization with two-Breit-Wigner-type resonances for the phenomenological spectral density that satisfies the low-energy theorem for the scalar form factor. Considering the uncertainties of the QCD parameters and the experimental masses and widths of the scalar resonances σ and $f_0(980)$, we obtain a prediction for light quark mass $m_q(2\ \mathrm{GeV}) = \frac{1}{2}(m_u(2\ \mathrm{GeV}) + m_d(2\ \mathrm{GeV})) = 4.7^{+0.8}_{-0.7}$ MeV, which is consistent with the Particle Data Group value and QCD sum rule determinations in the pseudoscalar channel. This agreement provides a consistent framework connecting QCD sum rules and low-energy hadronic physics. We also obtain the decay constants of σ and $f_0(980)$ at 2 GeV, which are approximately 0.64–0.83 and 0.40–0.48 GeV, respectively.

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I. INTRODUCTION

The light quark masses are fundamental parameters in QCD; thus, it is important to determine these parameters from different methods. Due to color confinement, the light quark masses cannot be measured from experiments directly. Therefore, their values are determined by relating the light quark masses to other physical quantities which can be obtained from theories or experiments. The main QCD-based methods for determining the light quark masses are lattice QCD (see, e.g., Ref. [1] for a review) and QCD sum rules (QCDSRs) [2–8].

The pion channel is the most common method to determine the light quark masses from QCDSRs. In Ref. [4], Bijnens *et al.* studied the value of the light quark mass combination $m_u + m_d$ in QCD using both finite-energy sum rules (FESRs) and Laplace sum rules (LSRs) for the divergence of the axial current with the quantum numbers of the pion, finding $m_u(1\ \mathrm{GeV}) + m_d(1\ \mathrm{GeV}) = 12 \pm 2.5$ MeV, which leads to a light quark mass $m_q(2\,\mathrm{GeV}) = \frac{1}{2}(m_u(2\,\mathrm{GeV}) + m_d(2\,\mathrm{GeV})) = 4.8 \pm 1.0$ MeV at the Particle Data Group (PDG) standard energy scale 2 GeV. Later, after including five-loop-order and higher-order quark-mass corrections to the correlation function of the same current, a more accurate result $m_q(2\ \mathrm{GeV}) = 4.1 \pm 0.2$ MeV was found by using FESRs [7].

In addition to the divergence of the axial current, one can also relate the light quark masses to other currents. It is clearly important to establish the self-consistency of the quark mass extracted from different channels. In Ref. [8], Cherry *et al.* used the $I=0$ scalar current to study this problem. By linking the phenomenological spectral density to the $\pi\pi$ scattering amplitude, they obtained the average light quark mass $m_q(1\ \mathrm{GeV}) = 5.2 \pm 0.6$ MeV. However, the main uncertainty in this analysis is determining the normalization between the theoretical and phenomenological spectral density. As discussed in Ref. [3], it is difficult to assess the hadronic uncertainties in Ref. [8], motivating our alternative approach. In this paper, we will reinvestigate the $I=0$ scalar channel using the improved Monte-Carlo-based QCD sum rule methodology recently proposed in Ref. [9]. After introducing a parametrization with two-Breit-Wigner-type resonances for the phenomenological spectral density normalized by the low-energy theorem, a Monte-Carlo-based analysis will be presented for the QCD sum rule master equation with the $I=0$ scalar current in the rigorous Hölder-inequality-determined sum rule window. Based on this analysis, we will give robust constraint on the light quark mass m_q and predictions for the decay constants of σ and $f_0(980)$.

II. QCD SUM RULE FOR $I=0$ SCALAR CHANNEL

We consider the correlation function

$$\Pi(q^2) = i\int d^4x e^{iqx}\langle 0|T j_s(x) j_s^\dagger(0)|0\rangle, \tag{1}$$

where $j_s = m_q\frac{1}{\sqrt{2}}(\bar{u}u + \bar{d}d)$ is the $I=0$ renormalization group invariant scalar current and $m_q = \frac{1}{2}(m_u + m_d)$ is the average mass of u and d quarks. The theoretical

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representation of this function has been calculated by using the operator product expansion (OPE) method [10–12]; however, it is believed that other nonperturbative contributions to the correlation function must be included, and thus we also should include the instanton contribution $\Pi^{(\mathrm{inst})}(q^2)$ in the theoretical representation of the correlation function [13–17].

To obtain a QCD sum rule, we first need to Borel-transform the theoretical representation of the correlation function, which gives [10–17]

$$
\begin{aligned}
R^{(\mathrm{theo})}(\tau,\hat{m}_q) &= \frac{1}{\tau}\hat{B}\Pi^{(\mathrm{OPE})}(q^2)+\frac{1}{\tau}\hat{B}\Pi^{(\mathrm{inst})}(q^2)\\
&= m_q^2(1/\sqrt{\tau})\cdot\left\{\frac{3}{8\pi^2}\left(1+\frac{17}{3}\frac{\alpha_s(1/\tau)}{\pi}\right)\frac{1}{\tau^2}+\frac{3}{8\pi^2}\frac{\alpha_s(1/\tau)}{\pi}\frac{2}{\tau^2}(\gamma_E-1)+\frac{\langle\alpha_s G^2\rangle}{8\pi}\left(1+\frac{11}{2}\frac{\alpha_s(1/\tau)}{\pi}\right)\right.\\
&\quad\left.+3\langle m_q\bar{q}q\rangle\left(1+\frac{13}{3}\frac{\alpha_s(1/\tau)}{\pi}\right)-\frac{176}{27}\pi\kappa\alpha_s\langle\bar{q}q\rangle^2\left[\frac{\alpha_s(1/\tau)}{\alpha_s(\mu_0^2)}\right]^{1/9}\tau+\frac{3}{8\pi^2}\frac{e^{\frac{-\rho^2}{2\tau}}\rho^2}{\tau^3}\left(K_0\left(\frac{\rho^2}{2\tau}\right)+K_1\left(\frac{\rho^2}{2\tau}\right)\right)\right\},
\end{aligned}
\tag{2}
$$

where $\hat{B}$ is the Borel transformation operator, $\alpha_s(1/\tau)=4\pi/(9\ln(1/(\tau\Lambda_{\mathrm{QCD}}^2)))$ is the running coupling constant for three flavors at scale $1/\sqrt{\tau}$ (the QCD scale $\Lambda_{\mathrm{QCD}}=0.353$ GeV [18]), κ is the vacuum factorization violation factor which parameterizes the deviation of the four-quark condensate from a product of two-quark condensates, ρ is the instanton size in the instanton liquid model, and K_0 and K_1 are modified Bessel functions. We have considered the renormalization group (RG) improvement of the sum rules [19] and anomalous dimensions for condensates [20,21] in Eq. (2), where μ_0 is the renormalization scale for condensates, and

$$
m_q(1/\sqrt{\tau})=\hat{m}_q\cdot\left[\frac{4\pi}{9\ln(\frac{1}{\tau\Lambda_{\mathrm{QCD}}^2})}\left(1-\frac{64}{81}\frac{\ln(\ln(\frac{1}{\tau\Lambda_{\mathrm{QCD}}^2}))}{\ln(\frac{1}{\tau\Lambda_{\mathrm{QCD}}})}\right)\right]^{4/9}
\tag{3}
$$

is the running light quark mass at scale $1/\sqrt{\tau}$ where $\hat{m}_q$ is the RG-invariant light quark mass. In Eq. (2), we also have included the α_s corrections to dimension-4 operators, which may play an important role in the determination of the QCD sum rule window from the Hölder inequality as in Ref. [9].

It is also necessary to construct a phenomenological spectral density model which is related to the correlation function through the dispersion relation integral. Considering the resonance nature of scalar mesons, we insert the lowest two-pion intermediate state,[1] as part of a complete set, into Eq. (1); i.e., by inserting $\int\frac{d^3\boldsymbol{k}_1}{(2\pi)^3 2E_{k_1}}\frac{d^3\boldsymbol{k}_2}{(2\pi)^3 2E_{k_2}}(|\pi^+(k_1)\pi^-(k_2)\rangle\langle\pi^+(k_1)\pi^-(k_2)|+\frac{1}{2!}|\pi^0(k_1)\pi^0(k_2)\rangle\langle\pi^0(k_1)\pi^0(k_2)|)+$ "other intermediate states" for the correlation function of current j_s and using Cutkosky's cutting rules [22], the phenomenological expression for $\mathrm{Im}\Pi(s)$ can then be found,

$$
\begin{aligned}
&\mathrm{Im}\Pi^{(\mathrm{phen})}(s)\\
&=\frac{3}{64\pi}\sqrt{1-\frac{4m_\pi^2}{s}}|F_s(s)|^2\\
&\quad+\text{contributions from excited states and continuum (ESC)},
\end{aligned}
\tag{4}
$$

where m_π is the mass of the pion, and $\langle 0|j_s(0)|\times\pi^+(k_1)\pi^-(k_2)\rangle=\frac{1}{\sqrt{2}}F_s((k_1+k_2)^2)$ has been used. We have classified all contributions from intermediate states other than the two-pion intermediate state, including those from the four-pion intermediate state, into contributions from ESC. According to chiral perturbative theory (ChPT), the scalar form factor $F_s(s)$ will be normalized by a low-energy theorem $F_s(0)=m_\pi^2$ [23], so we will constrain our phenomenological spectral density with this condition in the following.

In Ref. [8], the phenomenological spectral density for the $I=0$ scalar channel is related to the $\pi\pi$ scattering amplitude via the scalar form factor $F_s(s)$. However, because of a lack of experimental data consistent with ChPT at some energy scale, Cherry *et al.* introduced multiple assumptions for their phenomenological spectral density, which dominated the uncertainties in their analysis. In this paper, we will perform an independent analysis by parameterizing the phenomenological spectral density with the mass spectrum for the $I=0$ scalar channel directly and incorporate the ChPT low-energy theorem.

The $0^+(0^{++})$ meson spectra are rather crowded; there are too many particles with quantum numbers $0^+(0^{++})$ listed in the Review of Particle Physics [24] for a single nonet. Many different models have been used to describe the structures of these scalar mesons in QCDSRs, including

[1]There exist higher intermediate states which contain more particles, e.g., the four-pion intermediate state. However, multiple particle intermediate states would be kinetic suppressed by small phase-space factors; thus, we will classify these intermediate states together with other two particle intermediate states into "other intermediate states" below.

ordinary $\bar{q}q$ meson, four-quark state, glueball, and hybrid models [10,11,25–29]. However, the possible mixings between mesons with the same quantum numbers make this problem even more complex, and a widely accepted conclusion of research on the structures of these scalar mesons has not been achieved.

Among all these $I=0$ scalar mesons, we notice that both σ and $f_0(980)$ have the two-pion decay mode as their dominant decay mode. Thus, we can conjecture that there are contributions from poles of σ and $f_0(980)$ in the two-pion scalar form factor; i.e., $F_s(s)$ may have two poles at $s=m_\sigma - im_\sigma\Gamma_\sigma$ and $s=m_{f_0}-im_{f_0}\Gamma_{f_0}$, where m_σ and Γ_σ (m_{f_0} and Γ_{f_0}) are the mass and width of σ ($f_0(980)$) meson, respectively.

Considering the normalization of the form factor $|F_s(0)|^2=m_\pi^4$ from ChPT, we can construct a model with two Breit-Wigner-type resonances for the phenomenological spectral density which meets the above requirements as follows[2]:

$$\begin{aligned}\frac{1}{\pi}\mathrm{Im}\Pi^{(\mathrm{resonance})}(s) &= \frac{3}{64\pi^2}\cdot|F_s(s)|^2 \\ &= \frac{3}{64\pi^2}\cdot m_\pi^4\left(\beta\cdot\frac{m_\sigma^4+m_\sigma^2\Gamma_\sigma^2}{(s-m_\sigma^2)^2+m_\sigma^2\Gamma_\sigma^2}\right. \\ &\quad \left.+(1-\beta)\cdot\frac{m_{f_0}^4+m_{f_0}^2\Gamma_{f_0}^2}{(s-m_{f_0}^2)^2+m_{f_0}^2\Gamma_{f_0}^2}\right), \qquad (5)\end{aligned}$$

where we have omitted the small mass of pion ($m_\pi = 0.139$ GeV [24]) in the square root in Eq. (4). The parameter β ($0\le\beta\le 1$) describes the relative contribution of σ and $f_0(980)$ to the phenomenological spectral density in our model.

For the ESC contributions in the phenomenological spectral density, we still use the traditional ESC model, i.e.,

$$\begin{aligned}\frac{1}{\pi}\mathrm{Im}\Pi^{(\mathrm{ESC})}(s) = m_q^2(1/\sqrt{\tau})\cdot\Bigg(&\frac{3}{8\pi^2}\left(1+\frac{17}{3}\frac{\alpha_s}{\pi}\right)s \\ &-\frac{3}{4\pi^2}\frac{\alpha_s}{\pi}s\ln(s\tau) \\ &-\frac{3}{4\pi}sJ_1(\sqrt{s}\rho)Y_1(\sqrt{s}\rho)\Bigg)\theta(s-s_0), \qquad (6)\end{aligned}$$

where s_0 is the continuum threshold separating the contributions from excited states and continuum, and J_1 and Y_1 are Bessel function of the first and second kind, respectively.

[2]Notice that our model does not exclude other $0^+(0^{++})$ mesons from having a $\bar{q}q$-component; however, the contributions to the two-pion scalar form factor originate from heavier scalar mesons should be negligible because of the exponential suppression factor in the Borel-transformed dispersion relation integral, and the form factor will be suppressed by the small branching ratio of the two-pion decay mode.

Collecting Eqs. (5) and (6) together, we can obtain our phenomenological spectral density as follows:

$$\frac{1}{\pi}\mathrm{Im}\Pi^{(\mathrm{phen})}(s) = \frac{1}{\pi}\mathrm{Im}\Pi^{(\mathrm{resonance})}(s)+\frac{1}{\pi}\mathrm{Im}\Pi^{(\mathrm{ESC})}(s). \qquad (7)$$

Then, the phenomenological representation for the Borel-transformed correlation function can be obtained by using the dispersion relation

$$\begin{aligned}R^{(\mathrm{phen})}(\tau,s_0,\beta,\hat{m}_q) &= \frac{1}{\pi}\int_0^\infty e^{-s\tau}\mathrm{Im}\Pi^{(\mathrm{phen})}(s)ds \\ &= R^{(\mathrm{resonance})}(\tau,\beta)+R^{(\mathrm{ESC})}(\tau,s_0,\hat{m}_q). \qquad (8)\end{aligned}$$

Finally, the master equation for QCD sum rules can be obtained by demanding the equivalence between Eqs. (2) and (8),

$$R^{(\mathrm{theo})}(\tau,\hat{m}_q) = R^{(\mathrm{phen})}(\tau,s_0,\beta,\hat{m}_q), \qquad (9)$$

which can be used to obtain the predictions for s_0, β, and $\hat{m}_q$ providing we take the condensates and instanton size on the theoretical side as well as the physical parameters for σ and $f_0(980)$ on the phenomenological side as input parameters.[3]

Obviously, because of the truncation of OPE and the simplicity of the phenomenological spectral density, Eq. (9) cannot be valid for all τ; thus, one requires a sum rule window in which the validity of the master equation can be established. Benmerrouche *et al.* presented a method based on the Hölder inequality which provides fundamental constraints on QCD sum rules [30]. By placing the excited states and continuum contributions on the theoretical side, we obtain

$$\begin{aligned}R^{(\text{theo-ESC})}(\tau,s_0,\hat{m}_q) &\equiv R^{(\mathrm{theo})}(\tau,\hat{m}_q)-R^{(\mathrm{ESC})}(\tau,s_0,\hat{m}_q) \\ &= \frac{1}{\pi}\int_0^{s_0} e^{-s\tau}\mathrm{Im}\Pi^{(\mathrm{phen})}(s)ds. \qquad (10)\end{aligned}$$

Then, the Hölder inequality for QCD sum rules can be written as

[3]We can use Eq. (9) to obtain predictions for resonance parameters in our phenomenological spectral density as in Ref. [9], in principle. However, because the theoretical side of Eq. (9) is proportional to the square of the light quark mass m_q, the master equation is sensitive with the value of m_q; thus, a stable match between the two sides of the master equation is difficult to establish providing different input m_q. Conversely, by taking the resonance parameters as input parameters, we can use Eq. (9) to constrain the value of m_q effectively.

$$R^{(\text{theo-ESC})}(\omega\tau_1+(1-\omega)\tau_2,s_0,\hat{m}_q) \\ \leq [R^{(\text{theo-ESC})}(\tau_1,s_0,\hat{m}_q)]^{\omega}[R^{(\text{theo-ESC})}(\tau_2,s_0,\hat{m}_q)]^{1-\omega}, \tag{11}$$

where $0\leq\omega\leq 1$ and for parameters τ_1 and τ_2 we demand $\tau_1<\tau_2$. Notice that the different value of $\hat{m}_q$ does not change the allowed $(\tau,\,s_0)$ region from the Hölder inequality; thus, we can set any value for $\hat{m}_q$ in Eq. (11). Following Ref. [30], we will perform a local analysis on Eq. (11) with $\tau_2-\tau_1=\delta\tau=0.01\ \text{GeV}^{-2}$.

The only starting point of the Hölder inequality is that $\text{Im}\Pi^{(\text{phen})}(s)$ should be positive because of its relation to physical spectral functions; thus, Eq. (11) must be satisfied if sum rules are to consistently describe integrated physical spectral functions. In this paper, we will use the same iterative procedure to determine the sum rule window from the Hölder inequality rigorously as in Ref. [9], i.e., by choosing the maximally allowed region $[\tau_{\text{min}},\tau_{\text{max}}]$ of the Hölder inequality which is consistent with fitted s_0, where τ_{min} and τ_{max} are, respectively, the lower bound and upper bound of the allowed τ region.

In order to match the two sides of the master equation (9) in the sum rule window, a weighted-least-squares method [31] will be used in this paper. By randomly generating 200 sets of Gaussian distributed phenomenological input QCD parameters with given uncertainties (10% in this paper, which is the typical uncertainty in QCDSRs) at $\tau_j=\tau_{\text{min}}+(\tau_{\text{max}}-\tau_{\text{min}})\times(j-1)/(n_B-1)$, where $n_B=21$, we can estimate the standard deviation $\sigma_{\text{theo}}(\tau_j)$ for $R^{(\text{theo})}(\tau_j,\hat{m}_q)$.[4] Then, the phenomenological output parameters s_0, β, and $\hat{m}_q$ can be obtained by minimizing

$$\chi^2=\sum_{j=1}^{n_B}\frac{(R^{(\text{theo})}(\tau_j,\hat{m}_q)-R^{(\text{phen})}(\tau_j,s_0,\beta,\hat{m}_q))^2}{\sigma^2_{\text{theo}}(\tau_j)}. \tag{12}$$

III. NUMERICAL RESULTS

In the numerical analysis, we use the central values of input QCD parameters (at $\mu_0=1$ GeV) as follows [32,33]:

$$\langle\alpha_s G^2\rangle=0.07\ \text{GeV}^4,\qquad \langle m_q\bar{q}q\rangle=-(0.1\ \text{GeV})^4, \\ \kappa\alpha_s\langle\bar{q}q\rangle^2=\kappa\times 1.49\times 10^{-4}\ \text{GeV}^6,\qquad \rho=1/0.6\ \text{GeV}^{-1}. \tag{13}$$

The size of κ have been observed in different channels to be 2–4 [18,34,35]. Based on our previous study, $\kappa=2.8$ is the favored result in the vector channel with a traditional ESC model [9]. Although the factorization violation effect may differ between channels, it is still reasonable to assume the value of κ is in the region of 2–3 in the scalar channel, too. Thus, we consider $\kappa=2.0$ and $\kappa=3.0$ in our analysis and, as outlined below, we demonstrate that $\kappa\sim 2$ leads to greater agreement between our light quark mass predictions and the PDG value. In this paper, we will minimize the χ^2 with 1000 sets of Gaussian-distributed input QCD parameters listed in Eq. (13) with 10% uncertainties. Based on these 1000 fitting samples, we can obtain the median and the asymmetric standard deviations from the median for all output parameters; thus, we obtain the uncertainty originating from uncertainties of QCD parameters for s_0, β, and $\hat{m}_q$.[5]

In Fig. 1, we plot the allowed region for $(\tau,\,s_0)$ by the Hölder inequality for $\kappa=2.0$ and $\kappa=3.0$, respectively. From this figure, we find that the α_s corrections to $\langle\alpha_s G^2\rangle$ and $\langle m_q\bar{q}q\rangle$ extend the allowed region to a higher τ region and lower s_0 region as in the ρ channel [9], and the instanton contribution extends the allowed region further more. Thus both the α_s corrections to dimension-4 operators and the instanton contribution are important since we adopt the same iterative procedure as described in Ref. [9] to rigorously determine the sum rule window from the Hölder-inequality-allowed region.

Taking the experimental values of mass and width for σ and $f_0(980)$ [24]

$$m_\sigma=400\text{–}550\ \text{MeV},\qquad \Gamma_\sigma=400\text{–}700\ \text{MeV}, \\ m_{f_0}=990\pm 20\ \text{MeV},\qquad \Gamma_{f_0}=10\text{–}100\ \text{MeV} \tag{14}$$

as our input in the phenomenological spectral density model, we obtain different fitted s_0, β, and $\hat{m}_q$ by minimizing the corresponding χ^2 function. Detailed results are listed in Table I where we show the fitted results for $\kappa=2.0$ and $\kappa=3.0$, respectively. From this table we find that we can achieve very stable fits with $\kappa=2.0$; all uncertainties of output parameters are less than 10% providing 10% uncertainties of input QCD parameters. When we set $\kappa=3.0$, the uncertainty of $\hat{m}_q$ will reach to about 14%–18%, still in the accepted range of uncertainties for QCDSRs.

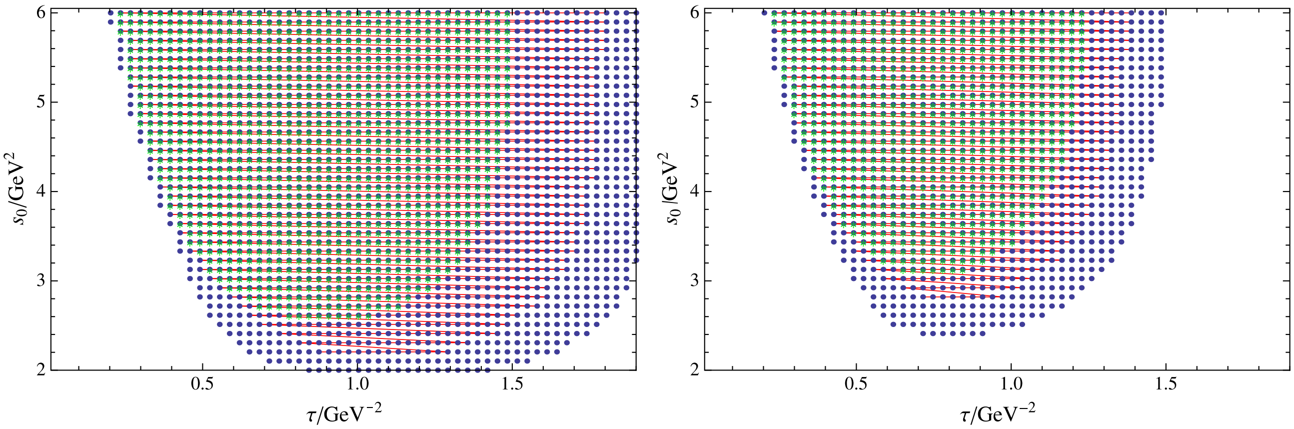
The suggested light quark mass at 2 GeV from PDG reads [24]

$$m_q^{\text{PDG}}(2\ \text{GeV})=\frac{1}{2}(m_u+m_d)=3.5^{+0.7}_{-0.3}\text{MeV}. \tag{15}$$

To compare our fitted results with $m_q^{\text{PDG}}(2\ \text{GeV})$, we also list the corresponding light quark mass at 2 GeV from our fitting procedure in Table I. Based on these data, we can obtain

[4]In practice, we will divide $R^{(\text{theo})}$ by $\hat{m}_q^2$ in order to remove the to-be-fitted parameter from the theoretical side; i.e., we estimate the standard deviation for $R^{(\text{theo})}(\tau_j,\hat{m}_q)/\hat{m}_q^2$.

[5]The mass and width of σ and $f_0(980)$ will be considered as fixed input parameters in each fit. However, we will input different combination of parameters for resonances based on experiment to estimate the uncertainties for output parameters which originate from parameters of resonances in the following.



(a) $\kappa = 2.0$ (b) $\kappa = 3.0$

FIG. 1. The region allowed by the Hölder inequality for (a) $\kappa = 2.0$ and (b) $\kappa = 3.0$. The region with (blue) dot or (red) line is allowed for sum rules with or without the instanton contribution, respectively. The region with (green) asterisk is allowed for sum rules without both the α_s corrections to dimension-4 operators and the instanton contribution.

$$m_q(2\ \mathrm{GeV}) = 4.1 \pm 0.4(\mathrm{resonance})^{+0.4}_{-0.3}(\mathrm{QCD})\ \mathrm{MeV} = 4.1^{+0.6}_{-0.5}\ \mathrm{MeV} \tag{16}$$

for $\kappa = 2.0$ and

$$m_q(2\ \mathrm{GeV}) = 5.3 \pm 0.6(\mathrm{resonance})^{+0.8}_{-0.5}(\mathrm{QCD})\ \mathrm{MeV} = 5.3^{+1.0}_{-0.8}\ \mathrm{MeV} \tag{17}$$

for $\kappa = 3.0$, where we report the average value of $m_q(2\ \mathrm{GeV})$ with different resonance parameters, and combine the standard deviation and the asymmetric standard deviation which originate from different resonance parameters and uncertainties of QCD input parameters, respectively. Comparison with the PDG tends to favor the smaller value of κ. However, since an exact value of κ not known, we use the average value for $\kappa = 2.0$ and $\kappa = 3.0$ as a conservative determination of our final result

TABLE I. Fitted results with different choices of the mass and width for the two resonances. All uncertainties of QCD input parameters listed in Eq. (13) are set to 10%.

	Inputs				Outputs			
	m_σ/MeV	Γ_σ/MeV	m_{f_0}/MeV	Γ_{f_0}/MeV	s_0/GeV^2	β	$\hat{m}_q$/MeV	$m_q(2\ \mathrm{GeV})$/MeV
$\kappa = 2.0$	400	400	990	100	$2.77^{+0.14}_{-0.16}$	$0.941^{+0.016}_{-0.023}$	$7.02^{+0.62}_{-0.44}$	$4.0^{+0.4}_{-0.3}$
	400	400	990	10	$2.71^{+0.13}_{-0.15}$	$0.995^{+0.001}_{-0.002}$	$6.87^{+0.54}_{-0.40}$	$4.0^{+0.3}_{-0.2}$
	400	700	990	100	$2.77^{+0.14}_{-0.16}$	$0.955^{+0.013}_{-0.020}$	$6.40^{+0.58}_{-0.41}$	$3.7^{+0.3}_{-0.2}$
	400	700	990	10	$2.71^{+0.13}_{-0.15}$	$0.996^{+0.001}_{-0.002}$	$6.25^{+0.50}_{-0.37}$	$3.6^{+0.3}_{-0.2}$
	550	400	990	100	$2.66^{+0.16}_{-0.20}$	$0.935^{+0.024}_{-0.033}$	$8.41^{+0.70}_{-0.51}$	$4.8^{+0.4}_{-0.3}$
	550	400	990	10	$2.60^{+0.15}_{-0.19}$	$0.995^{+0.002}_{-0.003}$	$8.35^{+0.67}_{-0.49}$	$4.8^{+0.4}_{-0.3}$
	550	700	990	100	$2.73^{+0.14}_{-0.16}$	$0.958^{+0.016}_{-0.024}$	$7.16^{+0.62}_{-0.44}$	$4.1^{+0.4}_{-0.3}$
	550	700	990	10	$2.68^{+0.14}_{-0.16}$	$0.996^{+0.001}_{-0.002}$	$7.06^{+0.57}_{-0.42}$	$4.1^{+0.3}_{-0.2}$
$\kappa = 3.0$	400	400	990	100	$3.03^{+0.09}_{-0.09}$	$0.872^{+0.030}_{-0.078}$	$9.00^{+1.60}_{-0.80}$	$5.2^{+0.9}_{-0.5}$
	400	400	990	10	$2.94^{+0.08}_{-0.09}$	$0.990^{+0.002}_{-0.005}$	$8.56^{+1.25}_{-0.69}$	$4.9^{+0.7}_{-0.4}$
	400	700	990	100	$3.03^{+0.09}_{-0.09}$	$0.896^{+0.026}_{-0.071}$	$8.28^{+1.54}_{-0.75}$	$4.8^{+0.9}_{-0.4}$
	400	700	990	10	$2.95^{+0.08}_{-0.08}$	$0.992^{+0.002}_{-0.004}$	$7.82^{+1.14}_{-0.63}$	$4.5^{+0.7}_{-0.4}$
	550	400	990	100	$2.99^{+0.10}_{-0.10}$	$0.835^{+0.041}_{-0.095}$	$10.7^{+1.6}_{-0.9}$	$6.2^{+0.9}_{-0.5}$
	550	400	990	10	$2.90^{+0.09}_{-0.10}$	$0.986^{+0.003}_{-0.008}$	$10.5^{+1.5}_{-0.8}$	$6.0^{+0.9}_{-0.5}$
	550	700	990	100	$3.03^{+0.09}_{-0.09}$	$0.881^{+0.032}_{-0.082}$	$9.27^{+1.61}_{-0.81}$	$5.3^{+0.9}_{-0.5}$
	550	700	990	10	$2.95^{+0.08}_{-0.08}$	$0.991^{+0.002}_{-0.005}$	$8.91^{+1.29}_{-0.71}$	$5.1^{+0.7}_{-0.4}$

$$m_q(2\ \mathrm{GeV}) = 4.7^{+0.8}_{-0.7}\ \mathrm{MeV}. \tag{18}$$

This central value result is slightly heavier than the PDG value in Eq. (15), but it is still consistent with it. We expect further experimental data on the mass and width for σ and $f_0(980)$ would reduce the uncertainty for our prediction.

From Table I, we also can obtain

$$\begin{aligned} s_0 &= 2.70 \pm 0.06(\mathrm{resonance})^{+0.14}_{-0.17}(\mathrm{QCD})\ \mathrm{GeV}^2 \\ &= 2.70^{+0.15}_{-0.18}\ \mathrm{GeV}^2 \end{aligned} \tag{19}$$

for $\kappa = 2.0$ and

$$\begin{aligned} s_0 &= 2.98 \pm 0.05(\mathrm{resonance})^{+0.09}_{-0.09}(\mathrm{QCD})\ \mathrm{GeV}^2 \\ &= 2.98^{+0.10}_{-0.10}\ \mathrm{GeV}^2 \end{aligned} \tag{20}$$

for $\kappa = 3.0$.

We notice that the uncertainties of the fitted continuum threshold s_0 are astonishing small, especially those originating from different resonance parameters. Krasnikov *et al.* pointed out that contributions from below the nth resonances and from above the $(n+1)$-th resonances in the spectral density can be separated by using $s_0 = \frac{1}{2}(m_n^2 + m_{n+1}^2)$, where m_n and m_{n+1} is the mass of the nth and $(n+1)$-th resonance, respectively [36]; i.e., s_0 is determined only by the mass positions of the two nearest resonances in the spectral density which are located at the two sides of s_0. If this choice for s_0 is also applicable in the present case, then we can give a simple explanation for why s_0 is not affected a lot by different resonance parameters: although we input different mass and width for σ and different width for $f_0(980)$, the mass of $f_0(980)$ is fixed, thus

$$s_0 = \frac{1}{2}(m_2^2 + m_3^2) \tag{21}$$

will not change significantly during our fitting procedure, where m_3 is the next excited state in the present scalar channel which couples with the scalar current j_s strongly. By using $m_2 = 990$ MeV from experiment and Eq. (21), we can estimate the mass for the next resonance, which ranges from 2.10 GeV ($\kappa = 2.0$) to 2.23 GeV ($\kappa = 3.0$). Based on the average value of m_3 which is about 2.17 GeV, $f_0(1370)$, $f_0(1500)$, and $f_0(1710)$ are sufficiently weakly coupled to j_s to be negligible. On the other hand, our result favors one resonance in the group of $f_0(2020)$, $f_0(2100)$, $f_0(2200)$, and $f_0(2330)$ [which are all $0^+(0^{++})$ resonances listed in the latest Review of Particle Physics [24]] for an appreciable coupling to j_s and the exponential suppression in the Laplace sum rule enables inclusion within the continuum.

The continuum threshold s_0 is introduced to separate out the contributions from excited states and continuum in the phenomenological spectral density. This expected purpose is achieved in many works of QCD sum rules under the narrow resonance approximation. However, we deal with resonances with nonzero width in the present case. Thus, there is a second possibility that we actually cannot separate the ESC contributions from the first several resonances contributions exactly because of the overlapping contributions from different resonances. If this is the case, then the traditional one-parameter (i.e., s_0) ESC model is too simple to describe the true physical spectral density. Although a large s_0 is obtained during the fitting procedure, which leads to $\sqrt{s_0} = 1.64$–1.73 GeV, we still cannot conclude that those scalar mesons between 1 and 2 GeV are excluded from the phenomenological spectral density. But, luckily, due to the heavier mass and relatively small two-pion decay branching ratio, the contributions from $f_0(1370)$ and $f_0(1500)$ are expected to be very small. For $f_0(1370)$, as an example, if we assume that there is a contribution from $f_0(1370)$ to the scalar form factor F_s, which has the same magnitude of contribution as $f_0(980)$ [obviously, the magnitude of $f_0(1370)$ is overestimated because the position of $f_0(1370)$ is further away from the normalization point of F_s, i.e., $s = 0$, than $f_0(980)$], then we can estimate a rough relative contribution from $f_0(1370)$ and $f_0(980)$ to the Borel-transformed correlation function in the whole sum rule window, which is about 20%–30%. After considering the relatively small two-pion decay branching ratio, the contribution from $f_0(1370)$ to the Borel-transformed correlation function will be at most at the same magnitude of the uncertainty of QCDSRs. Thus, the fitted light quark mass will not be affected a lot after including these contributions. However, to solve the s_0 problem comprehensively and rigorously, a better description of the ESC is deserved, which needs further study.

By extracting the coefficients for the two standard Breit-Wigner functions in the phenomenological spectral density in Eq. (7), we can define two effective coupling constants which describe the coupling between the scalar current j_s and the two resonances [σ and $f_0(980)$] as follows:

$$\lambda_\sigma = \beta \frac{3}{64\pi} m_\pi^4 (m_\sigma^2 + \Gamma_\sigma^2) \frac{m_\sigma}{\Gamma_\sigma}, \tag{22}$$

$$\lambda_{f_0} = (1-\beta) \frac{3}{64\pi} m_\pi^4 (m_{f_0}^2 + \Gamma_{f_0}^2) \frac{m_{f_0}}{\Gamma_{f_0}}. \tag{23}$$

These two effective coupling constants can be related to other physical quantities. By inserting one-particle intermediate states [σ and $f_0(980)$ states] as part of a complete set, $\int \frac{d^4 k}{(2\pi)^3 2E_k} (|\sigma(k)\rangle\langle\sigma(k)| + |f_0(980)(k)\rangle\langle f_0(980)(k)|) +$ "other intermediate states," into the correlation function (1), a traditional phenomenological density can be obtained,[6]

[6]We have extended the narrow resonances model with the Breit-Wigner resonances model for σ and $f_0(980)$.

TABLE II. Effective coupling constants and decay constants of σ and $f_0(980)$.

	m_σ/MeV	Γ_σ/MeV	m_{f_0}/MeV	Γ_{f_0}/MeV	$\lambda_\sigma/10^{-6}$ GeV^6	$f_\sigma(2\ \mathrm{GeV})$/GeV	$\lambda_{f_0}/10^{-6}$ GeV^6	$f_{f_0}(2\ \mathrm{GeV})$/GeV
$\kappa = 2.0$	400	400	990	100	1.68	0.81	3.22	0.45
	400	400	990	10	1.77	0.83	2.70	0.42
	400	700	990	100	1.98	0.95	2.46	0.43
	400	700	990	10	2.06	1.00	2.16	0.41
	550	400	990	100	3.31	0.69	3.55	0.40
	550	400	990	10	3.52	0.71	2.70	0.35
	550	700	990	100	3.32	0.81	2.29	0.37
	550	700	990	10	3.45	0.82	2.16	0.36
$\kappa = 3.0$	400	400	990	100	1.55	0.60	6.99	0.51
	400	400	990	10	1.76	0.68	5.41	0.48
	400	700	990	100	1.85	0.71	5.68	0.50
	400	700	990	10	2.05	0.80	4.32	0.47
	550	400	990	100	2.96	0.50	9.01	0.49
	550	400	990	10	3.49	0.57	7.57	0.46
	550	700	990	100	3.06	0.60	6.50	0.49
	550	700	990	10	3.44	0.66	4.86	0.44

$$\frac{1}{\pi}\mathrm{Im}\Pi^{(\mathrm{phen})}(s) = m_q^2 f_\sigma^2 m_\sigma^2 \cdot \frac{1}{\pi}\frac{m_\sigma \Gamma_\sigma}{(s-m_\sigma^2)^2 + m_\sigma^2\Gamma_\sigma^2} + m_q^2 f_{f_0}^2 m_{f_0}^2 \cdot \frac{1}{\pi}\frac{m_{f_0}\Gamma_{f_0}}{(s-m_{f_0}^2)^2 + m_{f_0}^2\Gamma_{f_0}^2} + \frac{1}{\pi}\mathrm{Im}\Pi^{(\mathrm{ESC})}(s), \tag{24}$$

where f_σ and f_{f_0} are the decay constants of σ and $f_0(980)$, respectively, which satisfy $\langle 0|\frac{1}{\sqrt{2}}(\bar{u}u + \bar{d}d)|\sigma\rangle = f_\sigma m_\sigma$ and $\langle 0|\frac{1}{\sqrt{2}}(\bar{u}u+\bar{d}d)|f_0(980)\rangle = f_{f_0} m_{f_0}$. Comparing Eq. (7) with Eq. (24), we can connect our effective coupling constants with f_σ and f_{f_0} as follows:

$$\lambda_\sigma = m_q^2(\mu) f_\sigma^2(\mu) m_\sigma^2, \tag{25}$$

$$\lambda_{f_0} = m_q^2(\mu) f_{f_0}^2(\mu) m_{f_0}^2, \tag{26}$$

where μ is an energy scale.

In Table II, we list the effective coupling constants and the decay constants of σ and $f_0(980)$ based on our fitted results listed in Table I. For simplicity, we only use the central values of the fitted β and $m_q(2\ \mathrm{GeV})$ to estimate the effective coupling constants and the decay constants, and we do not estimate the uncertainties for these constants. Based on our estimation, we obtain the average value $\bar{f}_\sigma(2\ \mathrm{GeV}) = 0.83$ GeV for $\kappa = 2.0$ and $\bar{f}_\sigma(2\ \mathrm{GeV}) = 0.64$ GeV for $\kappa = 3.0$, we may conclude that the value of the decay constant of σ at 2 GeV is around 0.64–0.83 GeV. In Ref. [37], Celenza *et al.* estimated the value of f_σ by using the Nambu–Jona-Lasinio (NJL) model; their result reads $f_\sigma(2\ \mathrm{GeV}) = 0.42$ GeV, 0.48 GeV, 0.35 GeV, and 0.43 GeV depending on different model parameters.[7] Our result, which favors a larger coupling between j_s and the σ state, is more consistent with the result from the linear sigma model ($L\sigma M$), which gives $f_\sigma(2\ \mathrm{GeV}) = 0.65$–$0.90$ GeV [38].[8] We also obtain $\bar{f}_{f_0}(2\ \mathrm{GeV}) = 0.40$ GeV for $\kappa = 2.0$ and $\bar{f}_{f_0}(2\ \mathrm{GeV}) = 0.48$ GeV for $\kappa = 3.0$; thus, the value of the decay constant of $f_0(980)$ at 2 GeV is about 0.40–0.48 GeV. It is interesting that our $f_0(980)$ decay constant agrees with Ref. [39], where $f_{f_0}(1\ \mathrm{GeV}) \simeq 0.35$ GeV and $f_{f_0}(2.1\ \mathrm{GeV}) \simeq 0.41$ GeV, considering the differences in our approaches.

We also tried to use a one-resonance model, i.e., set $\beta = 0$ or 1 in Eq. (5), to finish our fitting procedure. However, after including the constraint on the phenomenological spectral density from low-energy theorem, i.e., $|F_s(0)|^4 = m_\pi^4$, none of the combination of resonance mass and width based on Eq. (14) would lead to reasonable match between the two sides of the QCDSR master equation (9) in the QCD sum rule window allowed by the Hölder inequality. A simple explanation of this astonishing result is that the scalar form factor does receive contributions both from σ and $f_0(980)$ as we conjectured in the previous section.

Based on the above results, which lead to $\beta \sim 1$, it seems that the σ peak dominates the resonance contributions in the phenomenological spectral density; however, this expectation is not necessarily true, because of the large gap

[7] We have converted the value of f_σ at the momentum cutoff in the NJL model into the value of f_σ at 2 GeV.

[8] We use the result $\langle 0|m_q(\bar{u}u + \bar{d}d)|\sigma\rangle = f_\pi m_\pi^2$ from the linear sigma model, where $f_\pi = 93$ MeV is the pion decay constant, $m_q^{\mathrm{PDG}}(2\ \mathrm{GeV})$, and the mass of σ from experiment, to estimate $f_\sigma(2\ \mathrm{GeV})$.

between the peaks of σ and $f_0(980)$. Although the contribution from the σ peak dominates the low s region in the phenomenological spectral density, there is also a significant contribution from the $f_0(980)$ peak in the whole sum rule window. In fact, the total contribution from the σ peak to the Borel-transformed correlation function in the sum rule window, i.e., $\int_{\tau_{\min}}^{\tau_{\max}} R^{(\sigma\text{peak})}(\tau)d\tau$, can be about 46%–65% of total contributions from both the σ and $f_0(980)$ peaks with $\kappa = 2.0$. The specific percent changes as we input different mass and width parameters for the two resonances. For larger vacuum factorization violation factor, the contribution from σ will reduce. However, the existence of the enigmatic σ is still essential in our procedure with $\kappa = 3.0$.

Finally, the effects of the α_s corrections to dimension-4 operators and the instanton contribution are also studied. From Fig. 1 we have learned that without these effects, the allowed $\tau - s_0$ region would shrink; thus, it is more difficult to obtain an acceptable fitted result which is consistent with the Hölder inequality. In fact, we cannot obtain a stable fit with $\kappa = 3.0$ without these effects, and with $\kappa = 2.0$, we would obtain a fitted $\hat{m}_q$ [and $m_q(2\ \text{GeV})$] which is significantly larger than the physical value from PDG. Based on these results, we can conclude that both the α_s corrections to dimension-4 operators and the instanton contribution are essential contributions in the theoretical representation of the correlation function (1).

IV. CONCLUSIONS

In this paper, we have constructed a phenomenological spectral density model with two Breit-Wigner-type resonances [σ and $f_0(980)$] for the $I = 0$ scalar channel with a normalization constrained by the ChPT low-energy theorem, and conducted the sum rule analysis of this channel in the Hölder-inequality-determined sum rule window via the Monte-Carlo-based fitting procedure. Based on our analysis, we obtain a prediction for the light quark mass m_q using the experimental results for the masses and widths of σ and $f_0(980)$. The agreement between our result $m_q(2\ \text{GeV}) = 4.7^{+0.8}_{-0.7}$ MeV, the PDG value, and QCDSR determinations in the pion channel provide a consistent framework connecting QCD and low-energy hadronic physics (see also Ref. [40]). Furthermore, this agreement in the quark mass determinations confirms the validity of our improved Monte-Carlo-based QCD sum rules, which has previously been systematically examined in the ρ meson channel in Ref. [9]. Our results indicate both σ and $f_0(980)$ couple to the scalar current j_s strongly, i.e., both σ and $f_0(980)$ have a $\bar{q}q$-component.

The continuum threshold s_0 obtained from our fitting procedure seems to exclude scalar mesons between 1 and 2 GeV from the ESC contributions. There are two possibilities for understanding this result. One possibility is that those mesons are weakly coupled enough to be excluded from the phenomenological spectral density, and we expect the next excited state is in the group of scalar mesons which is heavier than 2 GeV and that the exponential suppression in the Laplace sum rule enables inclusion within the continuum. The other possibility is that the traditional ESC model is too simple to describe the true ESC contributions exactly, and we cannot use one parameter to separate ESC contributions from a spectral density with overlapping resonance contributions; thus, a more realistic ESC model including parameters other than s_0 is needed to solve this problem comprehensively and rigorously.

From our analysis, we also obtain the value of the decay constants of σ and $f_0(980)$ at 2 GeV, which are, respectively, around 0.64–0.83 and around 0.40–0.48 GeV. These two decay constants can be used in further studies on the decays of heavier mesons, e.g., B mesons, which can decay through the s-wave two-pion state.

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