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Reevaluation of neutron electric dipole moment with QCD sum rules

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We study the neutron electric dipole moment in the presence of the *CP*-violating operators up to dimension five in terms of the QCD sum rules. It is found that the operator product expansion calculation is robust when exploiting a particular interpolating field for a neutron, while there exist some uncertainties on the phenomenological side. By using input parameters obtained from the lattice calculation, we derive a conservative limit for the contributions of the *CP*-violating operators. We also show the detail of the derivation of the sum rules.

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I. INTRODUCTION

A variety of experimental efforts [1] has precisely determined the elements of the Cabibbo-Kobayashi-Maskawa (CKM) matrix [2,3], which is a source of *CP* violation in the standard model (SM). All of *CP*-violating processes ever observed are well-explained in terms of the single physical phase in the CKM matrix. The SM, which is based on the $SU(3)_C \times SU(2)_L \times U(1)_Y$ gauge symmetry, allows another *CP*-violating interaction: the θ term in the QCD sector. The *CP*-violating phenomena caused by the interaction are, however, quite different from those induced by the CKM phase; the QCD θ term gives rise to the *CP* violation in the flavor-conserving processes, while the CKM phase induces the *CP* violation in the flavor-changing ones. Furthermore, TeV-scale physics beyond the SM, such as the minimal supersymmetric standard model, often provides other *CP*-violating sources. In fact, additional *CP*-violating interactions are necessary from the cosmological point of view, since the observed baryon asymmetry in the Universe is not explained within the SM interactions.

The electric dipole moment (EDM) of the neutron is one of the physical quantities that are quite sensitive to the *CP* violation in the flavor-conserving interaction. Since there has been no experimental evidence for its existence so far, a severe constraint is imposed on the *CP*-violating interactions. The currently most stringent limit for the neutron EDM is given by the Institut Laue-Langevin experiment [4]:

$$|d_n| < 2.9 \times 10^{-26}\ e\,\mathrm{cm} \qquad (90\%\ \mathrm{C.L.}). \tag{1}$$

Moreover, several experimental projects which use ultracold neutrons are now under development and expected to have much improved sensitivities. For example, the nEDM Collaboration at the Paul Scherrer Institute [5] plans to deliver a sensitivity of $\sim 5 \times 10^{-27}\ e\,\mathrm{cm}$ and eventually to reach into the regime of $10^{-28}\ e\,\mathrm{cm}$. Similar sensitivities are expected to be achieved by the nEDM Collaboration at the Spallation Neutron Source at the U.S. Oak Ridge National Laboratory [6], the CryoEDM experiment [7], the NOP Collaboration at J-PARC [8], and the experiment at KEK-RCNP-TRIUMF [9]. Such high sensitivities provide an opportunity to probe the flavor-conserving *CP*-violating interactions in the TeV-scale physics beyond the SM. Furthermore, we may probe the flavor violation in the new physics indirectly. Even if the new flavor-violating interactions are introduced in the new physics, the relative *CP* phase between them and the CKM matrix may contribute to the EDM [10].

In order to translate the experimental limits for the neutron EDM into constraints on the *CP* violation on the Lagrangian at the parton level, one needs to obtain a relation between these two quantities. There are some attempts to derive the relation based on the naive dimensional analysis, the chiral perturbation theory, and the QCD sum rules, though they are considered to have large uncertainties. It is ultimately desired that the lattice QCD simulation would evaluate it in the future. There has been discussion of evaluation of the neutron EDM with lattice simulation [11].

In this work, we evaluate the neutron EDM with the QCD sum rules [12], including the *CP*-violating operators up to dimension five. It is considered that the QCD sum rules allow us to derive the relation more systematically than the naive dimensional analysis and the chiral perturbation theory [13]. Similar attempts have been already made in the previous works, e.g., in a series of papers by Pospelov and Ritz [14,15], and references therein. We also derive the sum rules for the neutron EDM, while we use the lattice QCD simulation result for the low-energy constant in the numerical evaluation of the neutron EDM. It is found that this gives a more conservative estimate than carrying out all of the evaluation within the framework of the QCD sum rules. This approach provides a way of eliminating theoretical errors from the calculation, while there still remains uncertainty resulting from the QCD sum rule technique itself.

This paper is organized as follows. In Sec. II, we review the CP-violating interactions at the parton level up to dimension five. From Sec. III, the analysis of the neutron EDM with the QCD sum rules starts. In Sec. III, we discuss phenomenological aspects of the correlator of the interpolating field to a neutron and, in Sec. IV, show the properties of the neutron-interpolating field. In Sec. V, the quark propagators are derived on the CP-violating and electromagnetic background. They are used to evaluate the operator product expansion (OPE) for the correlator in Sec. VI. The sum rules for the neutron EDM are derived in Sec. VII. We found that there is a difference between results in Refs. [14,15] and ours. In Sec. VIII, we extract the low-energy constant from the lattice QCD simulation result. In Sec. IX, our numerical results for the neutron EDM are derived. In Sec. X, the neutron EDM is discussed assuming that the Peccei-Quinn symmetry solves the strong CP problem [16]. Section XI is devoted to conclusion and discussion.

In the appendix, we show some useful formulas to derive the quark condensates in the CP-violating background. In Appendix A 1, we estimate the effect of the CP-violating interactions on the generic quark bilinear condensate $\langle 0|\bar{q}\Gamma q|0\rangle$, with Γ a 4×4 constant matrix, as well as on the quark and gluon background fields. In Appendix A 2, validity of the usage of the classical equations of motion of quarks in evaluation of the quark condensates is discussed. In Appendix A 3, the Wilson-line operators for the quark fields are discussed in the Fock-Schwinger gauge.

II. EFFECTIVE LAGRANGIAN

Let us first express the flavor-conserving CP-violating terms in the low-energy effective Lagrangian for the system consisting of light quarks and a gluon. We include all of the CP-violating operators up to dimension five:

$$\mathcal{L}_{\not{CP}} = -\sum_{q=u,d,s} m_q \bar{q} i\theta_q \gamma_5 q + \theta_G \frac{\alpha_s}{8\pi} G^A_{\mu\nu}\tilde{G}^{A\mu\nu} - \frac{i}{2}\sum_{q=u,d,s} d_q \bar{q}(F\cdot\sigma)\gamma_5 q - \frac{i}{2}\sum_{q=u,d,s}\tilde{d}_q \bar{q} g_s (G\cdot\sigma)\gamma_5 q. \tag{2}$$

Here, m_q represents the quark masses, $F_{\mu\nu}$ and $G^A_{\mu\nu}$ are the electromagnetic and gluon field strength tensors, respectively, g_s is the strong coupling constant ($\alpha_s = g_s^2/4\pi$), $F\cdot\sigma \equiv F_{\mu\nu}\sigma^{\mu\nu}$, $G\cdot\sigma \equiv G^A_{\mu\nu}\sigma^{\mu\nu}T^A$, and $\tilde{G}^A_{\mu\nu} \equiv \frac{1}{2}\epsilon_{\mu\nu\rho\sigma}G^{A\rho\sigma}$ with $\epsilon^{0123} = +1$. T^A denotes the generators in the $SU(3)_C$ algebra. The second, third, and fourth terms in Eq. (2) are called the effective QCD θ term and the electric and chromoelectric dipole moments (CEDMs) for quarks, respectively. The EDMs and CEDMs for quarks are dimension-five operators, and they are sensitive to the TeV-scale physics beyond the SM. The coefficients of the CP-violating operators (θ_q, θ_G, d_q, and $\tilde{d}_q$) are all assumed to be quite small, and we keep only the terms up to the first order of these parameters.

The first two terms in Eq. (2) are mutually related by the chiral rotation. Consider the following infinitesimal chiral rotation:

$$q \to q' = (1 - i\epsilon\rho_q\gamma_5)q, \tag{3}$$

where ϵ is an infinitesimal real constant and ρ_q are certain parameters for each quark. The Noether current associated with the transformation is given as

$$J_{5\mu} = \sum_{q=u,d,s}\rho_q\bar{q}\gamma_\mu\gamma_5 q. \tag{4}$$

The divergence of this current does not vanish. Instead,

$$\partial^\mu J_{5\mu} = \frac{\alpha_s}{4\pi}\Big(\sum_q \rho_q\Big) G^A_{\mu\nu}\tilde{G}^{A\mu\nu} + \sum_q 2im_q\rho_q\bar{q}\gamma_5(1+i\theta_q\gamma_5)q - \sum_q \rho_q[d_q\bar{q}(F\cdot\sigma)q + \tilde{d}_q\bar{q}g_s(G\cdot\sigma)q]. \tag{5}$$

Hereafter we choose ρ_q as

$$\rho_q = \theta_q/\theta_Q, \qquad \theta_Q \equiv \sum_{q=u,d,s}\theta_q. \tag{6}$$

Then, if we take the infinitesimal parameter in Eq. (3) as $\epsilon = \theta_Q/2$, the Lagrangian in Eq. (2) varies by

$$\delta\mathcal{L} = \partial^\mu J_{5\mu}\cdot\frac{\theta_Q}{2} = \sum_q m_q\bar{q}i\theta_q\gamma_5 q + \theta_Q\frac{\alpha_s}{8\pi}G^a_{\mu\nu}\tilde{G}^{a\mu\nu}, \tag{7}$$

which implies that

$$\mathcal{L}_{\not{CP}} \to \mathcal{L}'_{\not{CP}} = \bar{\theta}\frac{\alpha_s}{8\pi}G^A_{\mu\nu}\tilde{G}^{A\mu\nu} - \frac{i}{2}\sum_{q=u,d,s}d_q\bar{q}(F\cdot\sigma)\gamma_5 q - \frac{i}{2}\sum_{q=u,d,s}\tilde{d}_q\bar{q}g_s(G\cdot\sigma)\gamma_5 q, \tag{8}$$

where $\bar{\theta} = \theta_G + \theta_Q$.

Therefore, it is found that the γ_5-mass terms are always reduced to the ordinary ones, and it is $\bar{\theta}$ that is regarded as a physical parameter. Of course, one may in turn rotate out the θ term into the imaginary mass term through an appropriate chiral rotation.

In addition, there remains still some arbitrariness in the quark mass phases θ_q, since they are redefined into another through an $SU(3)$ chiral rotation. In this paper, we choose an appropriate set of θ_q so that the choice significantly reduces the CP-violating contribution to the vacuum expectation values of the quark bilinear. We take the condition in Ref. [17] to determine θ_q; that is, after the θ term rotated into the γ_5-mass term, the following relation should be satisfied:

$$\langle\Omega_{\not{CP}}|\mathcal{L}_{\not{CP}}|M^A\rangle = 0 \qquad (M^A = \pi, K, \eta). \tag{9}$$

The above condition is evaluated by using the partially conserved axial-vector current (PCAC) relations. In the current case, it is sufficient to examine the conditions for π^0 and η^0. By using the PCAC relations, one may readily deduce the conditions for the CP-violating parameters from Eq. (9):

$$\begin{aligned}\bar{\theta}(m_u\rho_u - m_d\rho_d) &= \tfrac{1}{2}m_0^2(\tilde{d}_u - \tilde{d}_d),\\ \bar{\theta}(m_u\rho_u + m_d\rho_d - 2m_s\rho_s) &= \tfrac{1}{2}m_0^2(\tilde{d}_u + \tilde{d}_d - 2\tilde{d}_s).\end{aligned} \tag{10}$$

In the calculation we parametrize the condensate $\langle\bar{q}g_s(G\cdot\sigma)q\rangle$ as [18]

$$\langle\bar{q}g_s(G\cdot\sigma)q\rangle = -m_0^2\langle\bar{q}q\rangle. \tag{11}$$

With the relation $\sum_q\rho_q = 1$, we then determine the quark mass phases as follows:

$$\begin{aligned}\rho_u &= \frac{m_*}{m_u}\left[1 + \frac{m_0^2}{2\bar{\theta}}\left\{\frac{\tilde{d}_u - \tilde{d}_d}{m_d} + \frac{\tilde{d}_u - \tilde{d}_s}{m_s}\right\}\right],\\ \rho_d &= \frac{m_*}{m_d}\left[1 + \frac{m_0^2}{2\bar{\theta}}\left\{\frac{\tilde{d}_d - \tilde{d}_u}{m_u} + \frac{\tilde{d}_d - \tilde{d}_s}{m_s}\right\}\right],\\ \rho_s &= \frac{m_*}{m_s}\left[1 + \frac{m_0^2}{2\bar{\theta}}\left\{\frac{\tilde{d}_s - \tilde{d}_u}{m_u} + \frac{\tilde{d}_s - \tilde{d}_d}{m_d}\right\}\right],\end{aligned} \tag{12}$$

where

$$m_* \equiv \frac{m_um_dm_s}{m_um_d + m_dm_s + m_um_s}. \tag{13}$$

III. PHENOMENOLOGICAL BEHAVIOR OF THE CORRELATOR

The QCD sum rules are based on an analysis of the correlator of interpolating fields.[1] In the method, OPE allows one to consistently separate the long- and short-distance contributions to the correlator, and the long-distance contributions are evaluated by condensations of quarks and a gluon. By comparing the evaluated correlator with the phenomenological model, the properties for the low-lying parts of the hadronic spectrum are derived. The Borel transformation is applied to the correlator there. In this section, we first discuss the phenomenological model for the correlator.

In the present case, the interpolating field must have the same quantum numbers as those of the neutron, and it is denoted by $\eta_n(x)$ hereafter. On a background with CP-violating sources, the matrix element of the interpolating field between the vacuum and the one-particle neutron state is given as

$$\langle\Omega_{\not{CP}}|\eta_n(x)|N_{\not{CP}}(\boldsymbol{p}, s)\rangle = Z_{n,\not{CP}}^{(1/2)}\cdot u_{n,CP}(\boldsymbol{p}, s)e^{-ip\cdot x}, \tag{14}$$

where $|\Omega_{\not{CP}}\rangle$ and $|N_{\not{CP}}(\boldsymbol{p}, s)\rangle$ indicate the vacuum and the one-particle neutron state on the CP-violating background, respectively. The spinor $u_{n,\not{CP}}(\boldsymbol{p}, s)$ is the on-shell neutron wave function which satisfies the Dirac equation:

$$(\not{p} - m_{n,\not{CP}}\cdot e^{-i\alpha_n\gamma_5})u_{n,\not{CP}}(\boldsymbol{p}, s) = 0. \tag{15}$$

Here we include a phase factor $e^{-i\alpha_n\gamma_5}$ into the mass term, which in general might appear as CP is broken in the vacuum. Since $Z_{n,\not{CP}}^{(1/2)}$ and $m_{n,\not{CP}}$ are both even in terms of the CP-violating parameters [11], up to the first order of them,

$$Z_{n,\not{CP}}^{(1/2)} = Z_n^{(1/2)}, \qquad m_{n,\not{CP}} = m_n, \tag{16}$$

where m_n is the mass of the neutron and $\lambda_n \equiv Z_n^{(1/2)}$ is the coupling between the physical neutron state and the interpolating field without CP-violating sources. Then the solution of Eq. (15) turns out to be

$$u_{n,\not{CP}}(\boldsymbol{p}, s) = e^{(i/2)\alpha_n\gamma_5}u_n(\boldsymbol{p}, s), \tag{17}$$

with $u_n(\boldsymbol{p}, s)$ an ordinary spinor wave function which satisfies $(\not{p} - m_n)u_n(\boldsymbol{p}, s) = 0$. As a result, Eq. (14) leads to

$$\langle\Omega_{\not{CP}}|\eta_n(x)|N_{\not{CP}}(\boldsymbol{p}, s)\rangle = \lambda_ne^{(i/2)\alpha_n\gamma_5}u_n(\boldsymbol{p}, s)e^{-ip\cdot x}. \tag{18}$$

The low-energy constant λ_n is to be determined later.

Now we analyze the correlator of the interpolating fields from the phenomenological viewpoint. It is defined as

$$\Pi(q) \equiv i\int d^4xe^{iq\cdot x}\langle\Omega_{\not{CP}}|T\{\eta_n(x)\bar{\eta}_n(0)\}|\Omega_{\not{CP}}\rangle_F, \tag{19}$$

where the subscript F implies that the correlator is evaluated on an electromagnetic field background. Our goal is to extract the EDM of the neutron from the correlator. The phase factor in Eq. (18), however, causes a mixture between electric and magnetic dipole moment structures and makes it difficult to pick out only the EDM from the QCD sum rules. So we first examine the Lorentz structures of the correlator and select a term independent of the phase α_n, i.e., chiral-invariant. As discussed in Ref. [14], up to the leading order on the background electromagnetic field, the correlator $\Pi(q)$ is estimated by inserting an effective vertex such as

$$\mathcal{L}_n = -\frac{i}{2}d_n\bar{N}(F\cdot\sigma)\gamma_5N = \frac{d_n}{2}\bar{N}\tilde{F}\cdot\sigma N. \tag{20}$$

Here, N [$\equiv N(x)$] denotes the renormalized neutron field which is approximately equivalent to $\lambda_n^{-1}e^{-i\alpha_n\gamma_5/2}\eta_n(x)$, and d_n is the EDM of the neutron. A similar procedure to those in Ref. [14] shows that terms with an odd number of Dirac matrices are independent of the phase factor α_n, and furthermore, those proportional to $\{\tilde{F}\cdot\sigma, \not{q}\}$ are the unique choice in this case. Therefore we focus only on such terms

[1]There are many review articles about the QCD sum rules. For example, see Ref. [19].

in the following calculation. Then, the phenomenological expression of the correlator is found to be[2]

$$\Pi^{(\mathrm{phen})}(q) = \tfrac{1}{2} f(q^2)\{\tilde{F}\cdot\sigma, \not{q}\} + \cdots, \tag{21}$$

where dots indicate terms with other Lorentz structures and

$$f(q^2) = \left(\frac{\lambda_n^2 d_n m_n}{(q^2 - m_n^2)^2} + \frac{A(q^2)}{q^2 - m_n^2} + B(q^2)\right) \tag{22}$$

with $A(q^2)$ and $B(q^2)$ functions which have no pole at $q^2 = m_n^2$. As noted in Ref. [14], since we are effectively dealing with a three-point function, it might be inconsistent to parametrize the continuum contribution in terms of a usual ansatz for the spectral function with a certain threshold in the QCD sum rules. We just neglect the contribution with expecting its significance to be small enough. Furthermore, we assume that the function $A(q^2)$ has little dependence on q^2 and regard it as a constant when we conduct the Borel transformation.

IV. NEUTRON-INTERPOLATING FIELD

In this section, we give a discussion on the choice of the neutron-interpolating field which we use for the QCD sum rule calculation. The field must have the same quantum numbers as the neutron. The most general interpolator for the neutron on the ordinary CP-even background is parametrized as

$$\eta_n(x) = j_1(x) + \beta j_2(x), \tag{23}$$

where

$$j_1(x) = 2\epsilon_{abc}(d_a^T(x) C\gamma_5 u_b(x)) d_c(x) \tag{24}$$

and

$$j_2(x) = 2\epsilon_{abc}(d_a^T(x) C u_b(x))\gamma_5 d_c(x). \tag{25}$$

Here the subscripts a, b, and c denote the color indices, and C is the charge conjugation matrix. The interpolator $j_1(x)$ is often used in lattice simulations. While $j_2(x)$ vanishes in the nonrelativistic limit, it should be included to the whole interpolating field since we deal with light quarks. The unphysical parameter β is to be fixed later so that the calculation is transparent.

When the calculation is carried out on the CP-violating background, however, the interpolating fields include additional components. This point is easily understood when one considers the chiral rotation discussed in Sec. II. As we have seen in Sec. II, the chiral rotation (3) transforms the Lagrangian $\mathcal{L}$ into another. The same transformation, in turn, changes the interpolators $j_1(x)$ and $j_2(x)$ into other ones as

$$\begin{aligned} j_1(x) &\to j_1(x) - i\epsilon[(\rho_u + \rho_d) i_1(x) + \rho_d i_2(x)],\\ j_2(x) &\to j_2(x) - i\epsilon[(\rho_u + \rho_d) i_2(x) + \rho_d i_1(x)], \end{aligned} \tag{26}$$

where

$$\begin{aligned} i_1(x) &= 2\epsilon_{abc}(d_a^T(x) C u_b(x)) d_c(x),\\ i_2(x) &= 2\epsilon_{abc}(d_a^T(x) C\gamma_5 u_b(x))\gamma_5 d_c(x). \end{aligned} \tag{27}$$

Therefore, with generic CP-violating terms as in Eq. (2), the interpolators acquire mixing terms as

$$\begin{aligned} \tilde{j}_1(x) &= j_1(x) + i\epsilon i_1(x) + i\delta i_2(x),\\ \tilde{j}_2(x) &= j_2(x) + i\epsilon i_2(x) + i\delta i_1(x),\\ \tilde{i}_1(x) &= i_1(x) + i\epsilon j_1(x) + i\delta j_2(x),\\ \tilde{i}_2(x) &= i_2(x) + i\epsilon j_2(x) + i\delta j_1(x), \end{aligned} \tag{28}$$

with ϵ and δ the small constants which are suppressed by the CP-violating parameters. Furthermore, the above expressions are rewritten as

$$\begin{aligned} \tilde{j}_1(x) &= (1 + i\delta\gamma_5)[j_1(x) + i\epsilon i_1(x)],\\ \tilde{j}_2(x) &= (1 + i\delta\gamma_5)[j_2(x) + i\epsilon i_2(x)],\\ \tilde{i}_1(x) &= (1 + i\delta\gamma_5)[i_1(x) + i\epsilon j_1(x)],\\ \tilde{i}_2(x) &= (1 + i\delta\gamma_5)[i_2(x) + i\epsilon j_2(x)], \end{aligned} \tag{29}$$

because

$$i_1(x) = \gamma_5 j_2(x), \qquad i_2(x) = \gamma_5 j_1(x). \tag{30}$$

Now that we concentrate on the chiral-invariant structure in the correlator of the neutron-interpolating field as discussed in Sec. III, the infinitesimal chiral rotation factor $(1 + i\delta\gamma_5)$ is ignorable. After all, the neutron-interpolating field which we deal with has the following structure:

$$\eta_n(x) = j_1(x) + \beta j_2(x) + i\epsilon[i_1(x) + \beta i_2(x)]. \tag{31}$$

The small constant ϵ is determined by the condition that the interpolating field $\eta_n(x)$ has a vanishing correlator with the current $\xi_n(x)$ defined as follows:

$$\xi_n(x) = i_1(x) + \beta i_2(x) + i\epsilon[j_1(x) + \beta j_2(x)]. \tag{32}$$

In what follows, however, we sweep away the contribution of the mixture terms in the interpolating field by choosing an appropriate value for the parameter β. In the subsequent sections, we calculate the correlator of $\eta_n(x)$ by using the OPE method. The correlator is expressed by the sum of the correlators for each component interpolator as

$$\begin{aligned} \langle\Omega_{\not{CP}}|T\{\eta_n(x)\bar{\eta}_n(0)\}|\Omega_{\not{CP}}\rangle_F &= \langle j_1, \bar{j}_1\rangle + \beta[\langle j_1, \bar{j}_2\rangle + \langle j_2, \bar{j}_1\rangle] + \beta^2\langle j_2, \bar{j}_2\rangle\\ &\quad + i\epsilon[\gamma_5\langle j_2, \bar{j}_1\rangle + \langle j_1, \bar{j}_2\rangle\gamma_5] + i\epsilon\beta[\{\langle j_1, \bar{j}_1\rangle, \gamma_5\}\\ &\quad + \{\langle j_2, \bar{j}_2\rangle, \gamma_5\}] + i\epsilon\beta^2[\gamma_5\langle j_1, \bar{j}_2\rangle + \langle j_2, \bar{j}_1\rangle\gamma_5], \end{aligned} \tag{33}$$

[2] In the published versions of Refs. [14,15], the coefficient of the double pole in Eq. (22) is different from ours by a factor of 2, while that in the revised arXiv versions is consistent with ours.

where

$$\langle a, \bar{b}\rangle \equiv \langle \Omega_{\not{CP}}|T\{a(x)\bar{b}(0)\}|\Omega_{\not{CP}}\rangle_F. \tag{34}$$

As discussed in Sec. III, we focus on parts of the correlators which have the Lorentz structures with an odd number of gamma matrices. Such terms anticommute with γ_5. Thus, in this case, the above expression leads to

$$\begin{aligned}\langle \Omega_{\not{CP}}|T\{\eta_n(x)\bar{\eta}_n(0)\}|\Omega_{\not{CP}}\rangle_F|_{\gamma\,\mathrm{odd}} &= \langle j_1, \bar{j}_1\rangle + \beta[\langle j_1, \bar{j}_2\rangle + \langle j_2, \bar{j}_1\rangle] + \beta^2\langle j_2, \bar{j}_2\rangle \\ &\quad + i\epsilon(1-\beta^2)[\langle j_1, \bar{j}_2\rangle - \langle j_2, \bar{j}_1\rangle]\gamma_5. \end{aligned}\tag{35}$$

This equation shows that the mixing terms in the interpolating field do not affect the correlator if one sets β to be ± 1. As we will see later, for our calculation, $\beta = +1$ is an appropriate choice, since this choice eliminates the subleading terms with an infrared logarithm, which yields ambiguity due to the infrared cutoff.[3] With this choice, one may simultaneously exclude the contribution of the mixing terms. Thus, we will not calculate such mixing contributions with keeping in mind that we will finally take $\beta = +1$ when we derive the QCD sum rules.[4] That is to say, we deal with the correlator

$$\begin{aligned}\langle \Omega_{\not{CP}}|T\{\eta_n(x)\bar{\eta}_n(0)\}|\Omega_{\not{CP}}\rangle_F &= \langle j_1, \bar{j}_1\rangle + \beta[\langle j_1, \bar{j}_2\rangle + \langle j_2, \bar{j}_1\rangle] + \beta^2\langle j_2, \bar{j}_2\rangle,\end{aligned}\tag{37}$$

and after the computation, we set $\beta = +1$.

V. QUARK PROPAGATORS ON THE *CP*-VIOLATING BACKGROUND

When evaluating the correlator (19) in the OPE, we need to obtain the quark propagators on the CP-violating background with an electromagnetic background field F. They are defined as follows:

$$[S^q_{ab}(x)]_{\alpha\beta} \equiv \langle \Omega_{\not{CP}}|T[q_{a\alpha}(x)\bar{q}_{b\beta}(0)]|\Omega_{\not{CP}}\rangle_F, \tag{38}$$

where α and β denote spinor indices. Expanding the propagators as

$$\begin{aligned}[S^q_{ab}(x)]_{\alpha\beta} &= [S^{q(0)}_{ab}(x)]_{\alpha\beta} + \chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0) \\ &\quad + [S^q_{ab}(x)]_{\alpha\beta}|_{1\mathrm{photon}} + [S^q_{ab}(x)]_{\alpha\beta}|_{1\mathrm{gluon}} + \cdots,\end{aligned}\tag{39}$$

we evaluate each term in x space. The first term is the free propagator, and the second term describes the correlator of the quark background fields, with $\chi^q_{a\alpha}(x)$ a classical Grassmann field which indicates the quark background field. The third and fourth terms represent the propagators including one photon and gluon, respectively. In the derivation of the quark propagators we use the classical equations of motion for quark fields given as

$$\begin{aligned}i\not{D}q &= m_q(1 + i\theta_q\gamma_5)q + \frac{i}{2}\sum_{q=u,d,s} d_q(F\cdot\sigma)\gamma_5 q \\ &\quad + \frac{i}{2}\sum_{q=u,d,s}\tilde{d}_q g_s(G\cdot\sigma)\gamma_5 q, \\ -i\bar{q}\overleftarrow{\not{D}} &= m_q\bar{q}(1 + i\theta_q\gamma_5) + \frac{i}{2}\sum_{q=u,d,s} d_q\bar{q}(F\cdot\sigma)\gamma_5 \\ &\quad + \frac{i}{2}\sum_{q=u,d,s}\tilde{d}_q g_s\bar{q}(G\cdot\sigma)\gamma_5,\end{aligned}\tag{40}$$

where $D_\mu = \partial_\mu - ie_qA_\mu - ig_sG^A_\mu T^A$ and $\bar{q}\overleftarrow{\not{D}} = \partial_\mu\bar{q}\gamma^\mu + ie_q\bar{q}\not{A} + ig_s\bar{q}\not{G}^AT^A$. The electromagnetic and gluon fields are denoted as A_μ and G^A_μ, respectively, with e_q the quark charge.

The first term in Eq. (39), $[S^{q(0)}_{ab}(x)]_{\alpha\beta}$, is readily evaluated by using the equations of motion without electromagnetic and gluon background fields. The result is

$$S^{q(0)}_{ab}(x) = \frac{i\delta_{ab}}{2\pi^2}\frac{\not{x}}{(x^2)^2} - \frac{m_q\delta_{ab}}{4\pi^2x^2}(1 - i\theta_q\gamma_5), \tag{41}$$

where we keep the terms up to the first order of the quark mass m_q.

Next, we evaluate the third and fourth terms in Eq. (39). These terms again are obtained from the equations of motion (40). In this calculation, it is convenient to use the Fock-Schwinger gauge [21] for both the electromagnetic and the gluon fields:

$$x^\mu A_\mu(x) = x^\mu G^A_\mu(x) = 0. \tag{42}$$

In this gauge, the fields are expanded by their field strength, such as

$$\begin{aligned}A_\mu(x) &= \frac{1}{2\cdot 0!}x^\nu F_{\nu\mu}(0) + \frac{1}{3\cdot 1!}x^\alpha x^\nu(D_\alpha F_{\nu\mu}(0)) \\ &\quad + \frac{1}{4\cdot 2!}x^\alpha x^\beta x^\nu(D_\alpha D_\beta F_{\nu\mu}(0)) + \cdots.\end{aligned}\tag{43}$$

By using the expression, the gauge covariant form of the propagators is obtained as follows:

$$\begin{aligned}S^q_{ab}(x)|_{1\mathrm{photon}} &= -\frac{ie_q}{32\pi^2}\delta_{ab}\left[\frac{1}{x^2}\{\not{x}, F\cdot\sigma\} - im_q(1 - i\theta_q\gamma_5)F\cdot\sigma\log(-\Lambda^2_{\mathrm{IR}}x^2)\right] \\ &\quad - \frac{d_q}{8\pi^2}\delta_{ab}\left[\frac{\not{x}\tilde{F}\cdot\sigma\not{x}}{(x^2)^2} + \frac{m_q}{2x^2}\{\not{x}, \tilde{F}\cdot\sigma\}\right],\end{aligned}\tag{44}$$

[3] The choice of β for the sum rules including only the QCD θ term is discussed in Ref. [20]. They argue that the optimal choice of β is $-1 \le \beta \le 0$ rather than 1, which is consistent with the conventional choices favored from a viewpoint of evaluation of λ_n. The discussion is, however, not applicable to the present case, since our sum rules contain several unknown parameters.

[4] The neutron-interpolating field for $\beta = +1$ is simply expressed as

$$\eta_n(x) = \tfrac{1}{2}\epsilon^{abc}(d^T_a C\sigma_{\mu\nu}d_b)\sigma^{\mu\nu}\gamma_5 u_c. \tag{36}$$

$$S^q_{ab}(x)|_{\mathrm{1gluon}} = -\frac{ig_s}{32\pi^2}\Big[\frac{1}{x^2}\{\not{x}, G_{ab}\cdot\sigma\} - im_q(1-i\theta_q\gamma_5)G_{ab}\cdot\sigma\log(-\Lambda_{\mathrm{IR}}^2x^2)\Big] - \frac{\tilde{d}_q g_s}{8\pi^2}\Big[\frac{\not{x}\tilde{G}_{ab}\cdot\sigma\not{x}}{(x^2)^2} + \frac{m_q}{2x^2}\{\not{x}, \tilde{G}_{ab}\cdot\sigma\}\Big], \tag{45}$$

with $G^{\mu\nu}_{ab} = G^{A\mu\nu}T^A_{ab}$. Here, a certain infrared (IR) cutoff Λ_{IR} is introduced in logarithmic terms. It was replaced to the quark masses when deriving the propagator from the equation motions. However, the contribution to the OPE with small quark momenta around the quark masses should not be included so that the IR cutoff is introduced.

Finally, we translate the quark and gluon background fields into their condensates. Here we just give resultant expressions for the relations between them. The details of the derivation is presented in Appendix A 1.

A single quark line, $\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0)$, is related with the quark condensate as

$$\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0) = \langle\Omega_{\not{C}\not{P}}|q_{a\alpha}(x)\bar{q}_{b\beta}(0)|\Omega_{\not{C}\not{P}}\rangle_F, \tag{46}$$

and it is to be expressed in terms of $\langle\bar{q}q\rangle$ as follows:

$$\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0) = -\frac{\delta_{ab}}{12}(1+i\theta_G\rho_q\gamma_5)_{\alpha\beta}\langle\bar{q}q\rangle + \frac{i}{48}\delta_{ab}\not{x}m_q\langle\bar{q}q\rangle - \frac{i}{96}\delta_{ab}\Big[\bar{\theta}m_q\rho_q e_q\chi + d_q + \Big(\kappa - \frac{1}{2}\xi\Big)e_q\tilde{d}_q\Big] \times\{\tilde{F}\cdot\sigma, \not{x}\}_{\alpha\beta}\langle\bar{q}q\rangle + \frac{i}{96}m_q e_q\chi\delta_{ab}\{F\cdot\sigma, \not{x}\}_{\alpha\beta}\langle\bar{q}q\rangle - \frac{i}{24}e_q\chi\delta_{ab}(\tilde{F}\cdot\sigma\gamma_5[1+i\rho_q\theta_G\gamma_5])_{\alpha\beta}\langle\bar{q}q\rangle. \tag{47}$$

Here, χ, κ, and ξ are the parameters for the quark condensates defined as [22]

$$\langle\bar{q}\sigma_{\mu\nu}q\rangle_F = e_q\chi F_{\mu\nu}\langle\bar{q}q\rangle, \tag{48}$$

$$g_s\langle\bar{q}G^A_{\mu\nu}T^Aq\rangle_F = e_q\kappa F_{\mu\nu}\langle\bar{q}q\rangle, \tag{49}$$

$$2g_s\langle\bar{q}\gamma_5\tilde{G}^A_{\mu\nu}T^Aq\rangle_F = ie_q\xi F_{\mu\nu}\langle\bar{q}q\rangle. \tag{50}$$

Also, in our calculation, we need the interaction part of the quark and gluon background fields,

$$g_s\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0)[G_{\mu\nu}]_{cd} = \langle g_s q_{a\alpha}(x)[G_{\mu\nu}]_{cd}\bar{q}_{b\beta}(0)\rangle_{F,\not{C}\not{P}}, \tag{51}$$

and it leads to the following equation:

$$g_s\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0)[G_{\mu\nu}]_{cd} = -\frac{1}{32}\Big(\delta_{ad}\delta_{bc} - \frac{1}{3}\delta_{ab}\delta_{cd}\Big)\langle\bar{q}q\rangle\Big[e_q\Big(\kappa F_{\mu\nu} - \frac{i}{2}\xi\tilde{F}_{\mu\nu}\gamma_5\Big)(1+i\theta_G\rho_q\gamma_5) - \frac{i}{4}m_q e_q\not{x}\Big(\kappa F_{\mu\nu} + \frac{1}{2}\bar{\theta}\rho_q\xi\tilde{F}_{\mu\nu}\Big) - \frac{i}{24}m_q m_0^2\epsilon_{\mu\nu\rho\sigma}x^\rho\gamma^\sigma\gamma_5 - \frac{i}{24}\bar{\theta}m_q\rho_q m_0^2(x_\mu\gamma_\nu\gamma_5 - x_\nu\gamma_\mu\gamma_5) - \frac{1}{12}m_0^2\sigma_{\mu\nu} - \frac{i}{12}m_0^2\theta_G\rho_q\sigma_{\mu\nu}\gamma_5\Big]_{\alpha\beta}. \tag{52}$$

VI. OPE ANALYSIS OF THE CORRELATOR

A. Leading order

Now we calculate the correlation function of the interpolating fields $\eta_n(x)$ in terms of the OPE. First, we carry out the leading-order calculation for the correlator

$$\Pi(x) = \langle\Omega_{\not{C}\not{P}}|T\{\eta_n(x)\bar{\eta}_n(0)\}|\Omega_{\not{C}\not{P}}\rangle_F. \tag{53}$$

As in Eq. (37), this correlator is decomposed into four correlators. We deal with them inclusively by using the following notation:

$$\Pi_{kl}(x) = \langle\Omega_{\not{C}\not{P}}|T\{j_k(x)\bar{j}_l(0)\}|\Omega_{\not{C}\not{P}}\rangle_F \qquad (k, l = 1, 2). \tag{54}$$

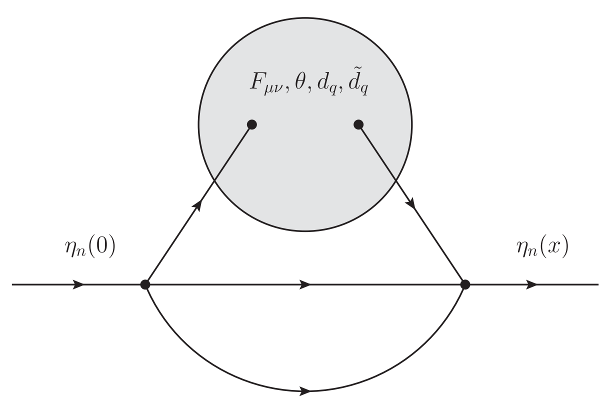

FIG. 1. Diagram which yields the leading contribution without emitting either a gluon or a photon.

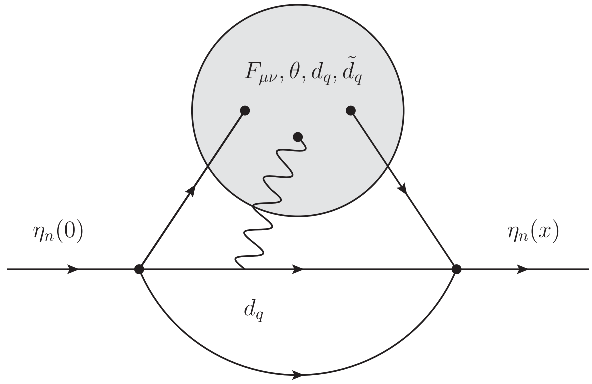

FIG. 2. Diagram which yields the leading and the next-to-leading-order contributions with emitting a photon. Those contributions vanish when $\beta = +1$.

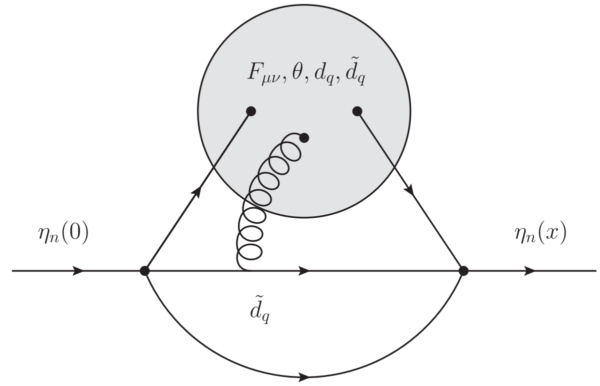

FIG. 3. Diagram which yields the leading and the next-to-leading-order contributions with emitting a gluon. Those contributions vanish when $\beta = +1$.

In Figs. 1–3, the diagrams which contribute to the correlators are illustrated. We denote each contribution to the correlators by the upper indices, i.e., $\Pi^{(I)}(x)$ or $\Pi^{(I)}_{kl}(x)$ with $I = 1, 2, 3$. From now on, we use the following abbreviation:

$$\bar{S}^{q}(x) \equiv C S^{qT}(x) C^{\dagger}, \tag{55}$$

with C the charge conjugation matrix.

Let us begin with evaluating $\Pi^{(1)}_{kl}(x)$. Each $\Pi^{(1)}_{kl}(x)$ is expressed in terms of the propagators $S^{q}_{ab}(x)$ as

$$\begin{aligned}
\Pi^{(1)}_{11}(x) &= 4\epsilon_{abc}\epsilon_{a'b'c'}\{-\mathrm{Tr}[\gamma_5 S^{u}_{ba'}(x)\gamma_5 \bar{S}^{d}_{ab'}(x)]S^{d}_{cc'}(x) + S^{d}_{cb'}(x)\gamma_5 \bar{S}^{u}_{ba'}(x)\gamma_5 S^{d}_{ac'}(x)\},\\
\Pi^{(1)}_{12}(x) &= 4\epsilon_{abc}\epsilon_{a'b'c'}\{-\mathrm{Tr}[\gamma_5 S^{u}_{ba'}(x)\bar{S}^{d}_{ab'}(x)]S^{d}_{cc'}(x)\gamma_5 + S^{d}_{cb'}(x)\bar{S}^{u}_{ba'}(x)\gamma_5 S^{d}_{ac'}(x)\gamma_5\},\\
\Pi^{(1)}_{21}(x) &= 4\epsilon_{abc}\epsilon_{a'b'c'}\{-\mathrm{Tr}[S^{u}_{ba'}(x)\gamma_5 \bar{S}^{d}_{ab'}(x)]\gamma_5 S^{d}_{cc'}(x) + \gamma_5 S^{d}_{cb'}(x)\gamma_5 \bar{S}^{u}_{ba'}(x) S^{d}_{ac'}(x)\},\\
\Pi^{(1)}_{22}(x) &= 4\epsilon_{abc}\epsilon_{a'b'c'}\{-\mathrm{Tr}[S^{u}_{ba'}(x)\bar{S}^{d}_{ab'}(x)]\gamma_5 S^{d}_{cc'}(x)\gamma_5 + \gamma_5 S^{d}_{cb'}(x)\bar{S}^{u}_{ba'}(x) S^{d}_{ac'}(x)\gamma_5\}.
\end{aligned} \tag{56}$$

When the propagators include neither a photon- nor gluon-emitting term, the expressions reduce to

$$\begin{aligned}
\Pi^{(1)}_{11}(x) &= 24\{\mathrm{Tr}[\gamma_5 S^{u}(x)\gamma_5 \bar{S}^{d}(x)]S^{d}(x) + S^{d}(x)\gamma_5 \bar{S}^{u}(x)\gamma_5 S^{d}(x)\},\\
\Pi^{(1)}_{12}(x) &= 24\{\mathrm{Tr}[\gamma_5 S^{u}(x)\bar{S}^{d}(x)]S^{d}(x)\gamma_5 + S^{d}(x)\bar{S}^{u}(x)\gamma_5 S^{d}(x)\gamma_5\},\\
\Pi^{(1)}_{21}(x) &= 24\{\mathrm{Tr}[S^{u}(x)\gamma_5 \bar{S}^{d}(x)]\gamma_5 S^{d}(x) + \gamma_5 S^{d}(x)\gamma_5 \bar{S}^{u}(x) S^{d}(x)\},\\
\Pi^{(1)}_{22}(x) &= 24\{\mathrm{Tr}[S^{u}(x)\bar{S}^{d}(x)]\gamma_5 S^{d}(x)\gamma_5 + \gamma_5 S^{d}(x)\bar{S}^{u}(x) S^{d}(x)\gamma_5\},
\end{aligned} \tag{57}$$

where

$$S^{q}_{ab}(x) = \delta_{ab} S^{q}(x). \tag{58}$$

As discussed in Sec. III, we focus on the terms proportional to $\{\tilde{F}\cdot\sigma, \not{q}\}$. For this reason we extract only the terms including $\{\tilde{F}\cdot\sigma, \not{x}\}$. They are found to be

$$\begin{aligned}
\Pi^{(1)}_{11}(x) &= \frac{i}{16\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}\bigg[(4e_d m_d \rho_d - e_u m_u \rho_u)\chi\bar{\theta} + \chi\{(e_d m_u \rho_u - e_u m_d \rho_d)\theta_Q + (e_u m_d \rho_u - e_d m_u \rho_d)\theta_G\}\\
&\quad + (6d_d - d_u) + \bigg(\kappa - \frac{1}{2}\xi\bigg)(6e_d \tilde{d}_d - e_u \tilde{d}_u)\bigg],\\
\Pi^{(1)}_{12}(x) &= \Pi^{(1)}_{21}(x) = \frac{i}{16\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}\bigg[(4e_d m_d \rho_d - e_u m_u \rho_u)\chi\bar{\theta} + (2d_d - d_u) + \bigg(\kappa - \frac{1}{2}\xi\bigg)(2e_d \tilde{d}_d - e_u \tilde{d}_u)\bigg],\\
\Pi^{(1)}_{22}(x) &= \frac{i}{16\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}\bigg[(4e_d m_d \rho_d - e_u m_u \rho_u)\chi\bar{\theta} + \chi\{(e_u m_d \rho_d - e_d m_u \rho_u)\theta_Q + (e_d m_u \rho_d - e_u m_d \rho_u)\theta_G\}\\
&\quad + (6d_d - d_u) + \bigg(\kappa - \frac{1}{2}\xi\bigg)(6e_d \tilde{d}_d - e_u \tilde{d}_u)\bigg].
\end{aligned} \tag{59}$$

Thus, $\Pi^{(1)}(x)$ is given as

$$\Pi^{(1)}(x) = \frac{i}{16\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}\bigg[(1+\beta)^2(4e_d m_d\rho_d - e_u m_u\rho_u)\chi\bar{\theta} + (1-\beta^2)\chi\{(e_d m_u\rho_u - e_u m_d\rho_d)\theta_Q + (e_u m_d\rho_u - e_d m_u\rho_d)\theta_G\} + 2(3+2\beta+3\beta^2)d_d - (1+\beta)^2 d_u + \left(\kappa - \frac{1}{2}\xi\right)\{2(3+2\beta+3\beta^2)e_d\tilde{d}_d - (1+\beta)^2 e_u\tilde{d}_u\}\bigg], \tag{60}$$

and for $\beta = +1$, the above expression reduces to

$$\Pi^{(1)}(x) = \frac{i}{4\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}\bigg[(4e_d m_d\rho_d - e_u m_u\rho_u)\chi\bar{\theta} + (4d_d - d_u) + \left(\kappa - \frac{1}{2}\xi\right)(4e_d\tilde{d}_d - e_u\tilde{d}_u)\bigg]. \tag{61}$$

Next, we evaluate $\Pi^{(2)}$. Here, we again use the expressions in Eq. (57), while one of the propagators in each correlator is $S^q(x)|_{1\text{photon}}$ in this case. The result is given as

$$\Pi^{(2)}_{11}(x) = \frac{i}{8\pi^4}(2d_d - d_u)\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}, \qquad \Pi^{(2)}_{12}(x) = \Pi^{(2)}_{21}(x) = -\frac{i}{8\pi^4}d_d\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\},$$
$$\Pi^{(2)}_{22}(x) = \frac{i}{8\pi^4}d_u\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}, \tag{62}$$

and they lead to

$$\Pi^{(2)}(x) = \frac{i}{8\pi^4}[2(1-\beta)d_d - (1-\beta^2)d_u]\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}. \tag{63}$$

Therefore, we find that $\Pi^{(2)}$ vanishes when we take $\beta = +1$:

$$\Pi^{(2)}(x) = 0. \tag{64}$$

Finally, we study $\Pi^{(3)}$. In this case, we use the equations in Eq. (56). By using Eq. (52), we find the resultant expressions as

$$\Pi^{(3)}_{11}(x) = \frac{i}{16\pi^4}\bigg[-e_d\tilde{d}_d\left(\kappa - \frac{1}{2}\xi\right) + (e_d\tilde{d}_u - e_u\tilde{d}_d)\left(\kappa + \frac{1}{2}\xi\right)\bigg]\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\},$$
$$\Pi^{(3)}_{12}(x) = \Pi^{(3)}_{21}(x) = \frac{i}{16\pi^4}e_d\tilde{d}_d\left(\kappa - \frac{1}{2}\xi\right)\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\},$$
$$\Pi^{(3)}_{22}(x) = \frac{i}{16\pi^4}\bigg[-e_d\tilde{d}_d\left(\kappa - \frac{1}{2}\xi\right) - (e_d\tilde{d}_u - e_u\tilde{d}_d)\left(\kappa + \frac{1}{2}\xi\right)\bigg]\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}. \tag{65}$$

Thus, $\Pi^{(3)}(x)$ is given as

$$\Pi^{(3)}(x) = \frac{i}{16\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}\bigg[-(1-\beta)^2\left(\kappa - \frac{1}{2}\xi\right)e_d\tilde{d}_d + (1-\beta^2)\left(\kappa + \frac{1}{2}\xi\right)(e_d\tilde{d}_u - e_u\tilde{d}_d)\bigg]. \tag{66}$$

Again, the correlator turns out to vanish for $\beta = +1$:

$$\Pi^{(3)}(x) = 0. \tag{67}$$

Taking the above discussion into account, we conclude that the correlator $\Pi(x)$ is given as

$$\Pi(x) = \frac{i}{16\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^3}\{\tilde{F}\cdot\sigma, \not{x}\}\bigg[(1+\beta)^2(4e_d m_d\rho_d - e_u m_u\rho_u)\chi\bar{\theta} + (1-\beta^2)\chi\{(e_d m_u\rho_u - e_u m_d\rho_d)\theta_Q + (e_u m_d\rho_u - e_d m_u\rho_d)\theta_G\} + (10+6\beta^2)d_d - (3+2\beta-\beta^2)d_u + \tilde{d}_d\bigg\{2\bigg[(3+2\beta+3\beta^2) - \frac{1}{2}(1-\beta)^2\bigg]e_d\left(\kappa - \frac{1}{2}\xi\right) - (1-\beta^2)e_u\left(\kappa + \frac{1}{2}\xi\right)\bigg\} + \tilde{d}_u\bigg\{(1-\beta^2)e_d\left(\kappa + \frac{1}{2}\xi\right) - (1+\beta)^2 e_u\left(\kappa - \frac{1}{2}\xi\right)\bigg\}\bigg], \tag{68}$$

and its Fourier transform is

$$\begin{aligned}\Pi(q) &= i\int d^4x e^{iq\cdot x}\Pi(x)\\ &= \frac{1}{64\pi^2}\langle\bar{q}q\rangle\log\left(\frac{-q^2}{\Lambda^2}\right)\{\tilde{F}\cdot\sigma, \not{q}\}\Big[(1+\beta)^2(4e_dm_d\rho_d - e_um_u\rho_u)\chi\bar{\theta} + (1-\beta^2)\chi\{(e_dm_u\rho_u - e_um_d\rho_d)\theta_Q\\ &\quad + (e_um_d\rho_u - e_dm_u\rho_d)\theta_G\} + (10+6\beta^2)d_d - (3+2\beta-\beta^2)d_u + \tilde{d}_d\Big\{2\Big[(3+2\beta+3\beta^2) - \frac{1}{2}(1-\beta)^2\Big]\\ &\quad \times e_d\left(\kappa - \frac{1}{2}\xi\right) - (1-\beta^2)e_u\left(\kappa+\frac{1}{2}\xi\right)\Big\} + \tilde{d}_u\Big\{(1-\beta^2)e_d\left(\kappa+\frac{1}{2}\xi\right) - (1+\beta)^2e_u\left(\kappa-\frac{1}{2}\xi\right)\Big\}\Big]. \end{aligned} \tag{69}$$

Here, a certain ultraviolet mass scale Λ is introduced, though it is irrelevant to our final result. When one sets $\beta = +1$, this expression reduces to

$$\Pi(q)^{(\mathrm{OPE})} = \frac{1}{16\pi^2}\langle\bar{q}q\rangle\log\left(\frac{-q^2}{\Lambda^2}\right)\{\tilde{F}\cdot\sigma,\not{q}\}\Big[(4e_dm_d\rho_d - e_um_u\rho_u)\chi\bar{\theta} + (4d_d - d_u) + \left(\kappa - \frac{1}{2}\xi\right)(4e_d\tilde{d}_d - e_u\tilde{d}_u)\Big]. \tag{70}$$

Equation (69) corresponds to Eqs. (9–12) in Ref. [15]. After taking $\beta = +1$, we find that the CEDM contribution, i.e., the last term in Eq. (70), differs from those in the reference by a factor of 4. In addition, the sign in front of ξ is opposite to the one in Ref. [15].

B. Next-to-leading order

Figures 2 and 3 yield the next-to-leading-order (NLO) contributions. By using the propagator given in Eq. (44), we evaluate the contribution by the diagram in Fig. 2 as

$$\begin{aligned}\Pi_{11}^{(2)}(x)_{\mathrm{NLO}} &= \frac{i}{32\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^2}\log(-\Lambda_{\mathrm{IR}}^2x^2)\{\tilde{F}\cdot\sigma,\not{x}\}[e_dm_d\rho_d\bar{\theta} + (e_um_u\rho_d - e_dm_d\rho_u)\theta_G + (e_dm_d\rho_d - e_um_u\rho_u)\theta_Q],\\ \Pi_{12}^{(2)}(x)_{\mathrm{NLO}} &= \Pi_{21}^{(2)}(x)_{\mathrm{NLO}} = -\frac{i}{32\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^2}\log(-\Lambda_{\mathrm{IR}}^2x^2)\{\tilde{F}\cdot\sigma,\not{x}\}e_dm_d\rho_d\bar{\theta},\\ \Pi_{22}^{(2)}(x)_{\mathrm{NLO}} &= \frac{i}{32\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^2}\log(-\Lambda_{\mathrm{IR}}^2x^2)\{\tilde{F}\cdot\sigma,\not{x}\}[e_dm_d\rho_d\bar{\theta} - (e_um_u\rho_d - e_dm_d\rho_u)\theta_G - (e_dm_d\rho_d - e_um_u\rho_u)\theta_Q],\end{aligned} \tag{71}$$

and therefore, $\Pi^{(2)}(x)_{\mathrm{NLO}}$ is found to be

$$\begin{aligned}\Pi^{(2)}(x)_{\mathrm{NLO}} &= \frac{i}{32\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^2}\log(-\Lambda_{\mathrm{IR}}^2x^2)\{\tilde{F}\cdot\sigma,\not{x}\}[(1-\beta)^2e_dm_d\rho_d\bar{\theta} + (1-\beta^2)\{(e_um_u\rho_d - e_dm_d\rho_u)\theta_G\\ &\quad + (e_dm_d\rho_d - e_um_u\rho_u)\theta_Q\}].\end{aligned} \tag{72}$$

The gluon contribution illustrated in Fig. 3 is also calculated by using the propagator displayed in Eq. (45). The resultant expressions are

$$\begin{aligned}\Pi_{11}^{(3)}(x)_{\mathrm{NLO}} &= -\frac{i}{64\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^2}\log(-\Lambda_{\mathrm{IR}}^2x^2)\{\tilde{F}\cdot\sigma,\not{x}\}\Big[e_dm_d\rho_d\left(\kappa+\frac{1}{2}\xi\right)\bar{\theta} + (e_dm_u\rho_d - e_um_d\rho_u)\left(\kappa-\frac{1}{2}\xi\right)\theta_G\\ &\quad + (e_um_d\rho_d - e_dm_u\rho_u)\left(\kappa-\frac{1}{2}\xi\right)\theta_Q\Big],\\ \Pi_{12}^{(3)}(x)_{\mathrm{NLO}} &= \Pi_{21}^{(3)}(x)_{\mathrm{NLO}} = \frac{i}{64\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^2}\log(-\Lambda_{\mathrm{IR}}^2x^2)\{\tilde{F}\cdot\sigma,\not{x}\}\bar{\theta}e_dm_d\rho_d\left(\kappa+\frac{1}{2}\xi\right),\\ \Pi_{22}^{(3)}(x)_{\mathrm{NLO}} &= -\frac{i}{64\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^2}\log(-\Lambda_{\mathrm{IR}}^2x^2)\{\tilde{F}\cdot\sigma,\not{x}\}\Big[e_dm_d\rho_d\left(\kappa+\frac{1}{2}\xi\right)\bar{\theta} - (e_dm_u\rho_d - e_um_d\rho_u)\left(\kappa-\frac{1}{2}\xi\right)\theta_G\\ &\quad - (e_um_d\rho_d - e_dm_u\rho_u)\left(\kappa-\frac{1}{2}\xi\right)\theta_Q\Big],\end{aligned} \tag{73}$$

and then,

$$\Pi^{(3)}(x)_{\rm NLO} = -\frac{i}{64\pi^4}\langle\bar{q}q\rangle\frac{1}{(x^2)^2}\log(-\Lambda_{\rm IR}^2x^2)\{\tilde{F}\cdot\sigma, \not{x}\}\bigg[(1-\beta)^2\bar{\theta}e_dm_d\rho_d\bigg(\kappa+\frac{1}{2}\xi\bigg) + (1-\beta^2)\{(e_dm_u\rho_d - e_um_d\rho_u)\theta_G + (e_um_d\rho_d - e_dm_u\rho_u)\theta_Q\}\bigg(\kappa-\frac{1}{2}\xi\bigg)\bigg]. \tag{74}$$

From the results in Eqs. (72) and (74), it is found that taking $\beta = +1$ makes the NLO contributions vanish, as mentioned before. Thus, we find that the correlator given in Eq. (70) is valid up to the next-to-leading order.

VII. QCD SUM RULES

In order to derive the QCD sum rules for the present case, we first extract the coefficient functions of $\{\tilde{F}\cdot\sigma, \not{q}\}$ from both the phenomenological and the OPE correlators, $\Pi^{(\rm phen)}$ in Eq. (21) and $\Pi^{(\rm OPE)}$ in Eq. (70), respectively:

$$C^{(\rm phen)}(Q^2) \equiv \frac{1}{2}\bigg[\frac{\lambda_n^2d_nm_n}{(Q^2+m_n^2)^2} - \frac{A}{Q^2+m_n^2}\bigg], \tag{75}$$

$$C^{(\rm OPE)}(Q^2) \equiv \frac{1}{16\pi^2}\langle\bar{q}q\rangle\Theta\log\bigg(\frac{Q^2}{\Lambda^2}\bigg), \tag{76}$$

with $Q^2 \equiv -q^2$ and

$$\Theta \equiv (4e_dm_d\rho_d - e_um_u\rho_u)\chi\bar{\theta} + (4d_d - d_u) + (\kappa - \tfrac{1}{2}\xi)(4e_d\tilde{d}_d - e_u\tilde{d}_u). \tag{77}$$

In Eq. (75), we neglect the continuum contribution and think of A as a constant, as discussed above. The QCD sum rules are obtained by equating the coefficient functions after the Borel transformation, i.e.,

$$\mathcal{B}[C^{(\rm phen)}(Q^2)] = \mathcal{B}[C^{(\rm OPE)}(Q^2)], \tag{78}$$

where the Borel transformation of the function $f(Q^2)$ is defined as

$$\mathcal{B}[f(Q^2)] \equiv \lim_{\substack{Q^2,n\to\infty\\ Q^2/n=M^2}} \frac{(Q^2)^{n+1}}{n!}\bigg(\frac{-d}{dQ^2}\bigg)^n f(Q^2), \tag{79}$$

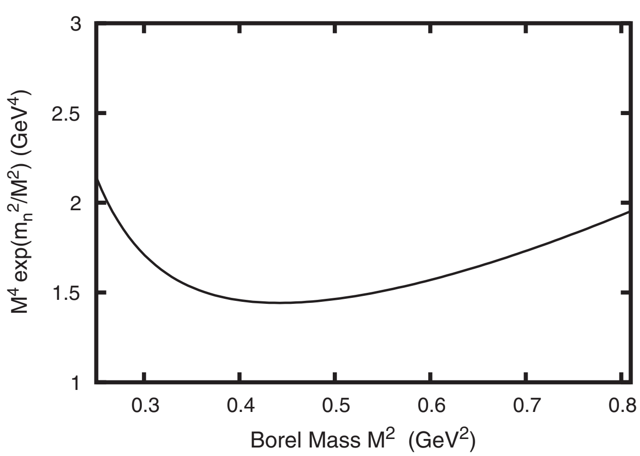

FIG. 4. Dependence of our sum rules on Borel mass M^2. The range of M is set to be 0.5 GeV $\leq M \leq$ 0.9 GeV.

with M so-called the Borel mass. Then, we finally derive the sum rules as follows:

$$\lambda_n^2d_nm_n - AM^2 = -\Theta\langle\bar{q}q\rangle\frac{M^4}{8\pi^2}e^{(m_n^2/M^2)}. \tag{80}$$

All we have to do is now reduced to determining the Borel mass M and the coupling λ_n, as well as estimating the parameter A.

To illustrate the dependence of the sum rules on the Borel mass, we plot $M^4e^{(m_n^2/M^2)}$, which is included in the right-hand side of Eq. (80), as a function of the Borel mass squared M^2 in Fig. 4. Here, the range of M is set to be 0.5 GeV $\leq M \leq$ 0.9 GeV. From the figure we find that the Borel mass dependence of our sum rule is moderate in the range of 0.6 GeV $\lesssim M \lesssim$ 0.8 GeV.

VIII. DETERMINATION OF λ_n FROM THE LATTICE

The low-energy constant λ_n determines the normalization of the QCD sum rules so that the uncertainties are directly linked to the final result. We extract its numerical value from the lattice QCD calculation presented in Ref. [23], in which the QCD matrix elements for the proton decay rate are evaluated. In fact, they evaluate a similar quantity for proton, though the isospin symmetry allows us to interpret it for the present purpose.

First, we introduce a generic notation for three-quark operators with an arbitrary spin structure:

$$\mathcal{O}^{\Gamma\Gamma'}(\boldsymbol{x}, t) \equiv \epsilon_{abc}[d_a^T(\boldsymbol{x}, t)C\Gamma u_b(\boldsymbol{x}, t)]\Gamma' d_c(\boldsymbol{x}, t), \tag{81}$$

with Γ and Γ' arbitrary 4×4 matrices. In the current case, the relevant matrices are $R = P_R \equiv \frac{1}{2}(1+\gamma_5)$ or $L = P_L \equiv \frac{1}{2}(1-\gamma_5)$. Now we define parameters α_1 and α_2 as follows:

$$\begin{aligned}\langle 0|\mathcal{O}^{RL}|N(\boldsymbol{p}, s)\rangle &= \alpha_1 P_L u_n(\boldsymbol{p}, s),\\ \langle 0|\mathcal{O}^{LL}|N(\boldsymbol{p}, s)\rangle &= \alpha_2 P_L u_n(\boldsymbol{p}, s).\end{aligned} \tag{82}$$

The phase definition is fixed such that α_1 and α_2 are both real and $\alpha_1 < 0$. The parity transformation of the above equations implies that

$$\begin{aligned}\langle 0|\mathcal{O}^{LR}|N(\boldsymbol{p}, s)\rangle &= -\alpha_1 P_R u_n(\boldsymbol{p}, s),\\ \langle 0|\mathcal{O}^{RR}|N(\boldsymbol{p}, s)\rangle &= -\alpha_2 P_R u_n(\boldsymbol{p}, s).\end{aligned} \tag{83}$$

The interpolating fields j_1 and j_2 are expressed in terms of the operators as

$$j_1(x) = 2(\mathcal{O}^{RL}(x) + \mathcal{O}^{RR}(x) - \mathcal{O}^{LL}(x) - \mathcal{O}^{LR}(x)), \tag{84}$$

$$j_2(x) = 2(\mathcal{O}^{LR}(x) - \mathcal{O}^{LL}(x) + \mathcal{O}^{RR}(x) - \mathcal{O}^{RL}(x)). \tag{85}$$

Thus their matrix elements between the vacuum and one-particle states are given as

$$\langle 0|j_1|N(\boldsymbol{p}, s)\rangle = 2(\alpha_1 - \alpha_2)u_n(\boldsymbol{p}, s), \tag{86}$$

$$\langle 0|j_2|N(\boldsymbol{p}, s)\rangle = -2(\alpha_1 + \alpha_2)u_n(\boldsymbol{p}, s), \tag{87}$$

and they lead to

$$\langle 0|\eta_n|N(\boldsymbol{p}, s)\rangle = 2[(\alpha_1 - \alpha_2) - \beta(\alpha_1 + \alpha_2)]u_n(\boldsymbol{p}, s). \tag{88}$$

From the equation we may relate λ_n with the parameters α_1 and α_2:

$$\lambda_n(\mu) = 2[(\alpha_1 - \alpha_2) - \beta(\alpha_1 + \alpha_2)], \tag{89}$$

with μ the renormalization scale. The parameters α_1 and α_2 at $\mu = 2$ GeV are estimated in Ref. [23] as

$$\alpha_1 = -0.0112 \pm 0.0012_{(\mathrm{stat})} \pm 0.0022_{(\mathrm{syst})}\ \mathrm{GeV}^3, \tag{90}$$

$$\alpha_2 = 0.0120 \pm 0.0013_{(\mathrm{stat})} \pm 0.0023_{(\mathrm{syst})}\ \mathrm{GeV}^3. \tag{91}$$

For $\beta = 1$, $\lambda_n(\mu = 2\ \mathrm{GeV})$ is given as

$$\begin{aligned}\lambda_n &= -4\alpha_2 \\ &= -0.0480 \pm 0.0052_{(\mathrm{stat})} \pm 0.0092_{(\mathrm{syst})}\ \mathrm{GeV}^3.\end{aligned} \tag{92}$$

Since the QCD parameter used here is evaluated at $\mu = 1$ GeV, we need to translate the above value of λ_n into that of $\mu = 1$ GeV. The one-loop correction for λ_n is

$$\begin{aligned}\lambda_n(\mu = 1\ \mathrm{GeV}) = \left(\frac{\alpha_s(1\ \mathrm{GeV})}{\alpha_s(m_c)}\right)^{-(2/9)}\left(\frac{\alpha_s(m_c)}{\alpha_s(2\ \mathrm{GeV})}\right)^{-(6/25)} \\ \times \lambda_n(\mu = 2\ \mathrm{GeV}),\end{aligned} \tag{93}$$

which results in a reduction factor of $\simeq 0.91$. As a result, we obtain

$$\lambda_n = -0.0436 \pm 0.0047_{(\mathrm{stat})} \pm 0.0084_{(\mathrm{syst})}\ \mathrm{GeV}^3 \tag{94}$$

for $\beta = +1$.

Let us compare the value of λ_n obtained here with those used in the previous works. In Ref. [14], for example, they exploit the values for λ_n evaluated in Ref. [24][5] by using the QCD sum rules. Two Dirac-γ structures, $\mathbb{1}$ and $\not{p}$, provide different sum rules. As evaluated in Ref. [24], these two sum rules yield relatively small values for λ_n; the lattice QCD value is several times larger than the values evaluated by using the QCD sum rules. The author in Ref. [24] also estimates the error for these values. It is about 30% for the sum rules result while 20% for the lattice QCD result. The lattice QCD result might have an uncertainty in the chiral extrapolation. Since there is no more guiding principle for judging which estimation is valid, we exploit the lattice QCD result in Eq. (94), because this choice leads to a rather conservative constraint for CP-violating sources.

[5]Note that the notation used in Ref. [24] is different from ours:

$$\lambda_n = 2\lambda_{\mathcal{O}} = \frac{2}{(2\pi)^2}\tilde{\lambda}_{\mathcal{O}}. \tag{95}$$

Also, notice that there is some difference between the results described in Ref. [24] and the corresponding expressions shown in Ref. [14].

IX. RESULTS

Now we estimate the neutron EDM by using the results obtained above. First of all, we rewrite the sum rules in Eq. (80) in a simple form:

$$c_0 + c_1 x = f(x), \tag{96}$$

where $x = M^2$ and

$$f(x) \equiv \frac{x^2}{8\pi^2}\exp\left(\frac{m_n^2}{x}\right), \qquad c_0 \equiv \frac{d_n\lambda_n^2 m_n}{-\Theta\langle\bar{q}q\rangle}, \qquad c_1 \equiv \frac{-A}{-\Theta\langle\bar{q}q\rangle}. \tag{97}$$

The right-hand side of Eq. (96) describes the behavior of the coefficient function obtained from the OPE calculation, while the left-hand side represents the phenomenological one. The first and second terms in the left-hand side correspond to the double and single pole contributions, i.e., the first and second terms in Eq. (22), respectively. Once given a Borel mass point $x = M^2$, one may readily pick out c_0 and c_1 from the tangent line to the function $f(x)$ at the point. Then, they are expressed as the functions of x as

$$\begin{aligned}c_0(x) &= \frac{1}{8\pi^2}(m_n^2 x - x^2)\exp\left(\frac{m_n^2}{x}\right), \\ c_1(x) &= \frac{1}{8\pi^2}(2x - m_n^2)\exp\left(\frac{m_n^2}{x}\right).\end{aligned} \tag{98}$$

From these expressions, it is found that the single pole contribution vanishes at $x = m_n^2/2$. Since the parameter A is unknown, this choice of x is favorable in order to estimate the double pole contribution. Then, at this point the value of c_0 is

$$c_0 = 1.8 \times 10^{-2} \quad (\text{for } x = m_n^2/2), \tag{99}$$

and, therefore, the neutron EDM d_n is evaluated as

$$d_n = \frac{-c_0\langle\bar{q}q\rangle}{\lambda_n^2 m_n}\Theta = 1.2 \times 10^{-1}\Theta. \tag{100}$$

Here we take $\langle\bar{q}q\rangle = -(0.225\ \mathrm{GeV})^3$.

The choice of the Borel mass, $M^2 = m_n^2/2$, is, however, quite arbitrary, and deviation from the above result due to the different choice of the Borel mass should be taken into account as a theoretical uncertainty. In Fig. 5, we plot the ratio of the single and double pole contributions as a function of M^2. From this figure, we find that the single pole contribution rapidly increases when the Borel mass is varied from $M^2 = m_n^2/2$. We here assume our sum rules to be valid within the region of the Borel mass in which the single pole contribution is less than 30% of the double pole contribution. This assumption leads to $0.36\ \mathrm{GeV}^2 < M^2 < 0.50\ \mathrm{GeV}^2$, and, in this region, d_n takes the following values:

$$d_n = 1.2^{+0.6}_{-0.3} \times 10^{-1}\Theta. \tag{101}$$

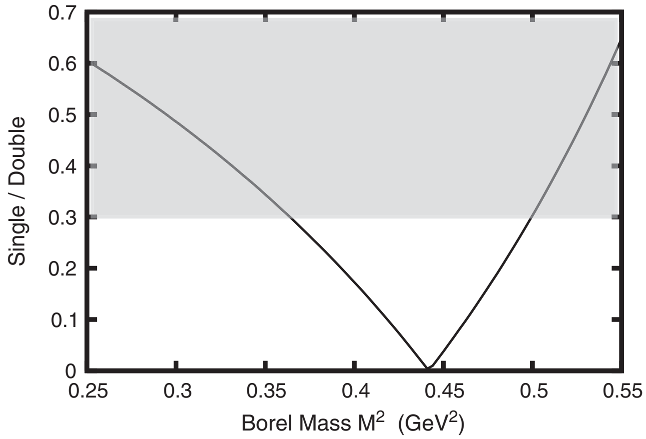

FIG. 5. Ratio of single and double pole contributions as a function of Borel mass M^2. The shaded region illustrates that single pole contribution is more than 30% of double pole contribution.

Here, the lower value corresponds to the upper limit of the Borel mass, and vice versa.

Next, we discuss the uncertainty of the OPE calculation. In this case, the truncation of the OPE leads to the uncertainty. Let us estimate it by evaluating the relative size of the higher-order contributions. Among them, the four-quark condensates such as $\langle \bar{q}q\bar{q}q\rangle$ are expected to yield sizable contributions, since they are free from loop suppression. On the assumption that these contributions vanish when one takes the quark masses to be zero, we expect that they are suppressed by at least a factor of $\langle \bar{q}q\rangle^{(2/3)}/M^2 \simeq 0.1$. Therefore, the uncertainty of the OPE calculation is estimated to be $\mathcal{O}(10)\%$.

Taking the above discussion into account, we finally evaluate the neutron EDM with theoretical uncertainty as follows:

$$d_n = 1.2^{+0.6}_{-0.3} \pm 0.1^{+0.7}_{-0.4} \times 10^{-1}\Theta, \qquad (102)$$

where the first uncertainty stems from the phenomenological calculation while the second one comes from the approximation in the OPE. We also include uncertainties originate from those in λ_n [see Eq. (94)], which is indicated by the third error in the above equation.[6] After all, it is found that there is almost an $\mathcal{O}(1)$ factor of uncertainty in our sum rule calculation.

Let us compare the result with those obtained by using the values of λ_n calculated with the QCD sum rules. In Ref. [22], the authors adopt $\lambda_n^2 = 1.05/(2\pi)^4\ \mathrm{GeV}^3$ for $\beta = -1$ from the QCD sum rules derived for the nucleon mass. The λ_n for $\beta = -1$ is equal to that for $\beta = 1$ in the nonrelativistic quark limit. In Ref. [25], it is shown that the neutron EDM prediction in the nonrelativistic quark model with the $SU(6)$ spin-flavor symmetry is derived in the QCD sum rules using the value of λ_n. By substituting the value into Eq. (100), one obtains $d_n = 3.3 \times 10^{-1}\Theta$. The "realistic" value of λ_n evaluated by the QCD sum rules in Ref. [24], $\lambda_n \simeq 0.022\ \mathrm{GeV}^3$, leads to a slightly larger result: $d_n = 4.6 \times 10^{-1}\Theta$. Thus, the overall factors of d_n of these results are several times larger than that of our result.

For convenience, we substitute the numerical values for the QCD parameters in Eq. (101). Here we take $m_0^2 = 0.8\ \mathrm{GeV}^2$, $\chi = -5.7 \pm 0.6\ \mathrm{GeV}^{-2}$, $\xi = -0.74 \pm 0.2$, and $\kappa = -0.34 \pm 0.1$ [18,26]. Then, with those parameters the center values, we find

$$d_n = 4.2 \times 10^{-17}\bar{\theta}[e\ \mathrm{cm}] + 0.47 d_d - 0.12 d_u + e(-0.18\tilde{d}_u + 0.18\tilde{d}_d - 0.008\tilde{d}_s). \qquad (103)$$

The contributions from $\bar{\theta}$ and the quark CEDMs to d_n may be changed furthermore by about $\pm 10\%$, mainly due to the theoretical uncertainty of χ.

X. UNDER THE PECCEI-QUINN SYMMETRY

It is known that $O(1)\ \bar{\theta}$ induces a too large neutron EDM, the strong *CP* problem. The Peccei-Quinn (PQ) symmetry is one of the solutions for the strong *CP* problem. If the PQ symmetry is introduced, $\bar{\theta}$ vanishes dynamically. However, if the quark CEDMs are nonvanishing, a linear term is induced to the axion potential [27],

$$V(\bar{\theta}) = K'\bar{\theta} - \tfrac{1}{2}K\bar{\theta}^2, \qquad (104)$$

where K is the topological susceptibility

$$K = -i\lim_{k\to 0} i\int d^4x e^{ikx}\left\langle T\left[\frac{\alpha_s}{8\pi}G\tilde{G}(x)\frac{\alpha_s}{8\pi}G\tilde{G}(0)\right]\right\rangle \qquad (105)$$

and K' is calculated by

$$K' = -i\lim_{k\to 0} i\int d^4x e^{ikx} \times \left\langle T\left[\frac{\alpha_s}{8\pi}G\tilde{G}(x)\frac{i}{2}\sum_{q=u,d,s}\tilde{d}_q\bar{q}g_s(G\cdot\sigma)\gamma_5 q(0)\right]\right\rangle. \qquad (106)$$

Minimizing the axion potential, an effective θ term is induced from the quark CEDM:

$$\bar{\theta}_{\mathrm{ind}} = -\frac{K'}{K} = \frac{m_0^2}{2}\sum_{q=u,d,s}\frac{\tilde{d}_q}{m_q}. \qquad (107)$$

Taking the induced θ term into account, the neutron EDM in the presence of the PQ symmetry is estimated as

$$d_n^{\mathrm{PQ}} = 1.2^{+0.6}_{-0.3} \pm 0.1^{+0.7}_{-0.4} \times 10^{-1}\Theta^{\mathrm{PQ}}, \qquad (108)$$

where

$$\Theta^{\mathrm{PQ}} = 4d_d - d_u + \left(\frac{m_0^2}{2}\chi + \kappa - \frac{1}{2}\xi\right)(4e_d\tilde{d}_d - e_u\tilde{d}_u). \qquad (109)$$

The contributions from the strange quark CEDM are canceled in the presence of the PQ symmetry [15]. Again, we

[6]We approximate the error in λ_n as the rms of the statistical and systematic errors displayed in Eq. (94).

substitute the numerical values for the QCD parameters as presented in the previous section. The result is

$$d_n^{\rm PQ} = 0.47 d_d - 0.12 d_u + e(0.35\tilde{d}_d + 0.17\tilde{d}_u). \quad (110)$$

XI. CONCLUSION AND DISCUSSION

We have studied the neutron EDM induced by the CP-violating interactions up to the dimension-five operators. In order to derive the relation between the CP-violating interactions and the neutron EDM, we have used the QCD sum rule technique. There are several phenomenological parameters to estimate the relation numerically. Pospelov and Ritz also analyzed the neutron EDM by using the QCD sum rules [14,15], and they determined the low-energy constant λ_n within the framework in the QCD sum rules. On the other hand, we have extracted the λ_n parameter from lattice calculations. This approach allows us to reduce a theoretical uncertainty and leads to a conservative constraint on the CP violations. Our result is about 70% smaller compared with the one obtained by Pospelov and Ritz. There still remains a sizable uncertainty resulting from the QCD sum rules itself due to a choice of the Borel mass scale. We have estimated the uncertainty from the Borel mass scale by assuming that the single pole contribution is less than 30% of the double pole contributions. This assumption leads to the theoretical error of about $\mathcal{O}(1)$.

Finally, we briefly comment on the contribution of the CP-violating dimension-six operators. Among the dimension-six operators, the following operator, called the Weinberg operator:

$$\mathcal{L}_{\not{CP}} = \tfrac{1}{3} w f_{ABC} G^A_{\mu\nu}\tilde{G}^{B\nu\lambda}G^{C\mu}_{\lambda},$$

might be comparable to the quark EDM and CEDM contributions, since they suffer from the chiral suppression. The other CP-violating dimension-six operators are effective four-quark operators of light quarks, which are negligible in the neutron EDM in typical high-energy models, since the Wilson coefficients are suppressed by the quark masses.[7] In our QCD sum rule calculation it is found that the contribution from the Weinberg operator is $\mathcal{O}(\langle\bar{q}q\rangle^2)$ and thus subdominant. There are a lot of discussions on the significance of the Weinberg operator [29], though no consensus has been reached yet.

ACKNOWLEDGMENTS

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APPENDIX

In this appendix, we list some techniques which we use to carry out the calculation.

1. Quark condensates on the *CP*-violating background

In this section, we discuss the effects of the CP-violating interactions on the quark condensates as well as on the quark and gluon background fields. We begin by estimating it for the generic quark bilinear condensate $\langle 0|\bar{q}\Gamma q|0\rangle$, with Γ a 4×4 constant matrix for which the quark bilinear $\bar{q}\Gamma q$ is an Hermitian operator. Then, by using the results obtained there, we derive the relations between the quark condensates and the background fields.

First, we evaluate the quark bilinear $\bar{q}\Gamma q$ on the CP-violating background. The contribution of the QCD θ term at the leading order is evaluated as [30]

$$\langle 0|\bar{q}\Gamma q|0\rangle_{\theta_G} = i\int d^4x \langle 0|T\{\bar{q}(0)\Gamma q(0)\theta_G \frac{\alpha_s}{8\pi} \times G^a_{\mu\nu}(x)\tilde{G}^{a\mu\nu}(x)\}|0\rangle + \mathcal{O}(\theta^2). \quad (A1)$$

Substituting Eq. (5) into the above expression, we obtain

$$\langle 0|\bar{q}\Gamma q|0\rangle_{\theta_G} = i\int d^4x\langle 0|T\Big\{\bar{q}(0)\Gamma q(0)\frac{\theta_G}{2}\Big[\partial^\mu J_{5\mu}(x) - 2i\sum_{q=u,d,s} m_q\rho_q\bar{q}(x)\gamma_5 q(x)\Big]\Big\}|0\rangle + \mathcal{O}(\theta^2), \quad (A2)$$

with $\rho_q = \theta_q/\theta_Q$. The first term in the equation is calculated with the aid of the integration by parts:

$$\begin{aligned} i\int d^4x\langle 0|T\Big\{\bar{q}(0)\Gamma q(0)\frac{\theta_G}{2}\partial^\mu J_{5\mu}(x)\Big\}|0\rangle &= -\frac{i\theta_G}{2}\int d^4x\langle 0|[J^0_5(x), \bar{q}(0)\Gamma q(0)]\delta(x^0)|0\rangle \\ &= \frac{i\theta_G}{2}\rho_q\langle 0|\bar{q}\{\gamma_5,\Gamma\}q|0\rangle. \end{aligned} \quad (A3)$$

For the second term, we insert the intermediate states and keep only the contributions of the one-particle states of the pseudo Nambu-Goldstone bosons π^0 and η^0:

$$\begin{aligned} -i\sum_{q=u,d,s}\int d^4x\langle 0|T\{\bar{q}(0)\Gamma q(0)\theta_G m_q\rho_q\bar{q}(x)i\gamma_5 q(x)\}|0\rangle &= -\frac{\theta_G}{f_\pi m_\pi^2}(m_u\rho_u - m_d\rho_d)\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\pi^0\rangle \\ &\quad -\frac{\theta_G}{\sqrt{3}f_\pi m_\eta^2}(m_u\rho_u + m_d\rho_d - 2m_s\rho_s)\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\eta^0\rangle, \end{aligned} \quad (A4)$$

[7] If the CP-violating four-quark operators include heavy quarks, the CEDMs for the light quarks and the Weinberg operators are radiatively induced by integration of the heavy quarks as shown in Ref. [28].

where f_π is the pion decay constant[8] and m_π and m_η denote the masses of π^0 and η^0, respectively.[9] As a result, we obtain

$$\begin{aligned}\langle 0|\bar{q}\Gamma q|0\rangle_{\theta_G} = &\frac{i\theta_G}{2}\rho_q\langle 0|\bar{q}\{\gamma_5,\Gamma\}q|0\rangle \\ &-\frac{\theta_G}{f_\pi m_\pi^2}(m_u\rho_u - m_d\rho_d)\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\pi^0\rangle \\ &-\frac{\theta_G}{\sqrt{3}f_\pi m_\eta^2}(m_u\rho_u + m_d\rho_d - 2m_s\rho_s) \\ &\times\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\eta^0\rangle. \end{aligned} \tag{A6}$$

Other contributions also may be evaluated through a similar procedure. For the contribution of the γ_5-mass terms,

$$\begin{aligned}\langle 0|\bar{q}\Gamma q|0\rangle_{\theta_q} = &-\frac{\theta_Q}{f_\pi m_\pi^2}(m_u\rho_u - m_d\rho_d)\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\pi^0\rangle \\ &-\frac{\theta_Q}{\sqrt{3}f_\pi m_\eta^2}(m_u\rho_u + m_d\rho_d - 2m_s\rho_s) \\ &\times\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\eta^0\rangle, \end{aligned} \tag{A7}$$

while for the contribution of the quark CEDM terms,

$$\begin{aligned}\langle 0|\bar{q}\Gamma q|0\rangle_{q\mathrm{CEDM}} = &\frac{1}{f_\pi m_\pi^2}\frac{m_0^2}{2}(\tilde{d}_u - \tilde{d}_d)\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\pi^0\rangle \\ &+\frac{1}{\sqrt{3}f_\pi m_\eta^2}\frac{m_0^2}{2}(\tilde{d}_u + \tilde{d}_d - 2\tilde{d}_s) \\ &\times\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\eta^0\rangle. \end{aligned} \tag{A8}$$

Furthermore, it is found that the quark EDMs induce no contribution.

Taking all of the contributions into account, we obtain the CP-violating contribution to the quark condensates as

$$\begin{aligned}&\langle 0|\bar{q}\Gamma q|0\rangle_{\not{CP}} \\ &= \frac{i\theta_G}{2}\rho_q\langle 0|\bar{q}\{\gamma_5,\Gamma\}q|0\rangle + \frac{1}{f_\pi m_\pi^2}\Big[\frac{m_0^2}{2}(\tilde{d}_u - \tilde{d}_d) \\ &\quad - \bar{\theta}(m_u\rho_u - m_d\rho_d)\Big]\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\pi^0\rangle \\ &\quad + \frac{1}{\sqrt{3}f_\pi m_\eta^2}\Big[\frac{m_0^2}{2}(\tilde{d}_u + \tilde{d}_d - 2\tilde{d}_s) \\ &\quad - \bar{\theta}(m_u\rho_u + m_d\rho_d - 2m_s\rho_s)\Big]\langle\bar{q}q\rangle\langle 0|\bar{q}\Gamma q|\eta^0\rangle \\ &= \frac{i\theta_G}{2}\rho_q\langle 0|\bar{q}\{\gamma_5,\Gamma\}q|0\rangle. \end{aligned} \tag{A9}$$

[8]We use the PCAC relation for π^0,

$$\partial_\mu J_A^\mu(x) = -f_\pi m_\pi^2\pi(x), \tag{A5}$$

and a similar relation for η^0.

[9]The effect of the π^0-η^0 mixing is suppressed by a small factor of $(m_u - m_d)/m_s$, and we ignore it for brevity.

Here, the second equality comes from the conditions in Eq. (10). Thus, the choice of the quark mass phases in Eq. (12) reduces the contribution of the CP-violating interactions to the vacuum condensates into a quite simple expression.

Note that the CP-violating contribution to the quark condensates vanishes in the basis where the θ term is completely rotated out into the imaginary mass term. Thus, the choice of this basis, which is often adopted in the chiral Lagrangian approach, simplifies the calculation. In our paper, however, we remain in a general basis in order to display each contribution explicitly.

Next, we discuss the way of translating the quark and gluon background fields into their condensates. To begin with, we consider a single quark line $\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0)$. In this case, it is related with the quark condensate as follows:

$$\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0) = \langle\Omega_{\not{CP}}|q_{a\alpha}(x)\bar{q}_{b\beta}(0)|\Omega_{\not{CP}}\rangle_F. \tag{A10}$$

Using the Fierz identity, the right-hand side of the expression leads to

$$\begin{aligned}&\langle\Omega_{\not{CP}}|q_{a\alpha}(x)\bar{q}_{b\beta}(0)|\Omega_{\not{CP}}\rangle_F \\ &= -\frac{\delta_{ab}}{12}\Big[\langle\bar{q}(0)q(x)\rangle_{F,\not{CP}} + \gamma_5\langle\bar{q}(0)\gamma_5 q(x)\rangle_{F,\not{CP}} \\ &\quad + \gamma^\mu\langle\bar{q}(0)\gamma_\mu q(x)\rangle_{F,\not{CP}} - \gamma^\mu\gamma_5\langle\bar{q}(0)\gamma_\mu\gamma_5 q(x)\rangle_{F,\not{CP}} \\ &\quad + \frac{1}{2}\sigma^{\mu\nu}\langle\bar{q}(0)\sigma_{\mu\nu}q(x)\rangle_{F,\not{CP}}\Big]_{\alpha\beta}. \end{aligned} \tag{A11}$$

These quark condensate terms are evaluated by conducting the short-distance expansion of the quark field in the Fock-Schwinger gauge as

$$q(x) = q(0) + x^\mu D_\mu q(0) + \cdots. \tag{A12}$$

We note that in this gauge one does not need to care about Wilson-line operators for the quark fields. (See Appendix A 3.)

In the case of CP-even vacuum, the Lorentz and CP invariance of vacuum tell us that

$$\langle\bar{q}\gamma_5 q\rangle = \langle\bar{q}\gamma_\mu q\rangle = \langle\bar{q}\gamma_\mu\gamma_5 q\rangle = 0. \tag{A13}$$

On the other hand, on an electromagnetic background, $\langle\bar{q}\sigma_{\mu\nu}q\rangle$ may have a nonzero vacuum expectation value proportional to the electromagnetic field strength $F_{\mu\nu}$. The electromagnetic field dependence for quark condensates is given as

$$\langle\bar{q}\sigma_{\mu\nu}q\rangle_F = \chi_q F_{\mu\nu}\langle\bar{q}q\rangle, \tag{A14}$$

where χ_q is called the quark condensate magnetic susceptibility [22]. Similar parametrization is used for the condensates including the gluon background field:

$$g_s\langle\bar{q}G^A_{\mu\nu}T^A q\rangle_F = \kappa_q F_{\mu\nu}\langle\bar{q}q\rangle, \tag{A15}$$

$$2g_s\langle\bar{q}\gamma_5\tilde{G}^A_{\mu\nu}T^A q\rangle_F = i\xi_q F_{\mu\nu}\langle\bar{q}q\rangle. \tag{A16}$$

As in Ref. [22], we assume χ_q, κ_q, and ξ_q to be proportional to the quark charge:

$$\chi_q = e_q\chi, \qquad \kappa_q = e_q\kappa, \qquad \xi_q = e_q\xi. \tag{A17}$$

This assumption corresponds to neglecting of the closed-loop contribution with gluon exchange.

Now let us consider the effect of the CP-violating interaction in Eq. (2) to the quark condensates. By using Eq. (A9) and the expansion in Eq. (A12), we evaluate each quark condensate on the CP-violating background as follows (with omitting the subscriptions F and $\not{CP}$ for simplicity as long as it is not confusing):

$$\langle\bar{q}(0)q(x)\rangle = \langle\bar{q}q\rangle, \tag{A18}$$

$$\langle\bar{q}(0)\gamma_5 q(x)\rangle = \langle\bar{q}\gamma_5 q\rangle_{\not{CP}} = i\theta_{G\rho q}\langle\bar{q}q\rangle, \tag{A19}$$

$$\begin{aligned}\langle\bar{q}(0)\gamma_\mu q(x)\rangle &= x^\nu\langle\bar{q}\gamma_\mu D_\nu q\rangle \\ &= \frac{1}{2}x^\nu\langle\bar{q}\{\gamma_\mu D_\nu + \gamma_\nu D_\mu\}q\rangle \\ &\quad + \frac{1}{2}x^\nu\langle\bar{q}\{\gamma_\mu D_\nu - \gamma_\nu D_\mu\}q\rangle \\ &= \frac{1}{4}x^\nu g_{\mu\nu}\langle\bar{q}\not{D}q\rangle + \frac{i}{4}x^\nu\langle\bar{q}\not{D},\sigma_{\mu\nu}]q\rangle \\ &= -\frac{i}{4}m_q x_\mu\langle\bar{q}q\rangle,\end{aligned} \tag{A20}$$

where we use the classical equations of motion in the quark condensates and move the covariant derivatives with help of total derivative. The validity of this procedure is discussed in Appendix A 2. Furthermore,

$$\begin{aligned}\langle\bar{q}(0)\gamma_\mu\gamma_5 q(x)\rangle &= x^\nu\langle\bar{q}\gamma_\mu D_\nu\gamma_5 q\rangle \\ &= \frac{1}{4}x^\nu g_{\mu\nu}\langle\bar{q}\not{D}\gamma_5 q\rangle + \frac{i}{4}x^\nu\langle\bar{q}[\not{D},\sigma_{\mu\nu}]\gamma_5 q\rangle \\ &= \frac{i}{2}m_q e_q\chi(\bar{\theta}\rho_q F_{\mu\nu} + \tilde{F}_{\mu\nu})x^\nu\langle\bar{q}q\rangle \\ &\quad + \frac{i}{2}\left(d_q + \left[\kappa - \frac{1}{2}\xi\right]e_q\tilde{d}_q\right)x^\nu F_{\mu\nu}\langle\bar{q}q\rangle,\end{aligned} \tag{A21}$$

and

$$\begin{aligned}\langle\bar{q}(0)\sigma_{\mu\nu}q(x)\rangle &= \langle\bar{q}\sigma_{\mu\nu}q\rangle \\ &= \langle\bar{q}\sigma_{\mu\nu}q\rangle_{CP\,\text{even}} + \langle\bar{q}\sigma_{\mu\nu}q\rangle_{\not{CP}} \\ &= e_q\chi[F_{\mu\nu} - \theta_G\rho_q\tilde{F}_{\mu\nu}]\langle\bar{q}q\rangle.\end{aligned} \tag{A22}$$

Taking the above discussion into account and using the relation

$$F_{\mu\nu}x^\mu\gamma^\nu\gamma_5 = +\tfrac{1}{4}\{\tilde{F}\cdot\sigma,\not{x}\} \tag{A23}$$

and

$$F\cdot\sigma = i\tilde{F}\cdot\sigma\gamma_5, \tag{A24}$$

we finally obtain the expression for the single quark line as follows:

$$\begin{aligned}\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0) = &-\frac{\delta_{ab}}{12}(1 + i\theta_G\rho_q\gamma_5)_{\alpha\beta}\langle\bar{q}q\rangle + \frac{i}{48}\delta_{ab}\not{x}_{\alpha\beta}m_q\langle\bar{q}q\rangle - \frac{i}{96}\delta_{ab}\left[\bar{\theta}m_q\rho_q e_q\chi + d_q + \left(\kappa - \frac{1}{2}\xi\right)e_q\tilde{d}_q\right] \\ &\times\{\tilde{F}\cdot\sigma,\not{x}\}_{\alpha\beta}\langle\bar{q}q\rangle + \frac{i}{96}m_q e_q\chi\delta_{ab}\{F\cdot\sigma,\not{x}\}_{\alpha\beta}\langle\bar{q}q\rangle - \frac{i}{24}e_q\chi\delta_{ab}(\tilde{F}\cdot\sigma\gamma_5[1 + i\rho_q\theta_G\gamma_5])_{\alpha\beta}\langle\bar{q}q\rangle.\end{aligned} \tag{A25}$$

Last, we evaluate the interaction part of the quark and gluon background fields:

$$g_s\chi^q_{a\alpha}(x)\chi^{-q}_{b\beta}(0)[G_{\mu\nu}]_{cd} = \langle g_s q_{a\alpha}(x)[G_{\mu\nu}]_{cd}\bar{q}_{b\beta}(0)\rangle_{F,\not{CP}}. \tag{A26}$$

Again, we use the Fierz identity and the short-distance expansion of the quark field, and through a similar calculation, we find the following results:

$$\begin{aligned}g_s\chi^q_{a\alpha}(x)\bar{\chi}^q_{b\beta}(0)[G_{\mu\nu}]_{cd} = &-\frac{1}{32}\left(\delta_{ad}\delta_{bc} - \frac{1}{3}\delta_{ab}\delta_{cd}\right)\langle\bar{q}q\rangle\times\left[e_q\left(\kappa F_{\mu\nu} - \frac{i}{2}\xi\tilde{F}_{\mu\nu}\gamma_5\right)(1 + i\theta_G\rho_q\gamma_5)\right. \\ &- \frac{i}{4}m_q e_q\not{x}\left(\kappa F_{\mu\nu} + \frac{1}{2}\bar{\theta}\rho_q\xi\tilde{F}_{\mu\nu}\right) - \frac{i}{24}m_q m_0^2\epsilon_{\mu\nu\rho\sigma}x^\rho\gamma^\sigma\gamma_5 - \frac{i}{24}\bar{\theta}m_q\rho_q m_0^2(x_\mu\gamma_\nu\gamma_5 - x_\nu\gamma_\mu\gamma_5) \\ &\left.- \frac{1}{12}m_0^2\sigma_{\mu\nu} - \frac{i}{12}m_0^2\theta_G\rho_q\sigma_{\mu\nu}\gamma_5\right]_{\alpha\beta}.\end{aligned} \tag{A27}$$

2. EQUATIONS OF MOTION

Let us discuss the validity of using classical equations of motion for quark condensates. We investigate the following quantity:

$$\langle 0|\bar{q}\Gamma(i\not{D} - m_q)q|0\rangle_\theta, \tag{A28}$$

where Γ is a (c-number) 4×4 matrix. The subscript indicates that this quantity is evaluated in the θ vacuum. One may readily generalize the discussion here for the case with other CP-violating sources. The discussion presented in this section is based on Ref. [31].

First, we define the generating functional $Z[\eta]_\theta$ on the same background:

$$Z[\eta]_\theta \equiv \int \mathcal{D}\bar{q}\mathcal{D}q \exp\left[i\int d^4x\{\mathcal{L} + \eta\bar{q}\Gamma(i\not{D} - m_q)q\}\right]. \tag{A29}$$

Here, the Lagrangian density $\mathcal{L}$ is

$$\mathcal{L} = \bar{q}(i\not{D} - m_q)q. \tag{A30}$$

The functional derivative of the generating function with respect to the function η yields Eq. (A28), that is,

$$\langle 0|\bar{q}\Gamma(i\not{D} - m_q)q|0\rangle_\theta \propto \frac{\delta Z[\eta]_\theta}{\delta\eta(0)}\bigg|_{\eta=0}. \tag{A31}$$

Now we replace the integration variable $\bar{q}$ with a new integration variable $\bar{q}'$ as

$$\bar{q} \to \bar{q}' = \bar{q} - \eta\bar{q}\Gamma. \tag{A32}$$

Since this step does not change the integral, then we obtain

$$Z[\eta] = \int \mathcal{D}\bar{q}\mathcal{D}q\left[\mathrm{Det}\left\{\frac{\delta\bar{q}'}{\delta\bar{q}}\right\}\right]^{-1}\exp\left[i\int d^4x\mathcal{L} + \mathcal{O}(\eta^2)\right], \tag{A33}$$

where the inverse of the Jacobian comes from the transformation of the measure for the fermionic variable.

Next, we evaluate the Jacobian in the expression above. Since we are interested in the first-order derivative of the generating function, we expand the Jacobian in η and keep only terms linear in η:

$$\frac{\delta\bar{q}'_\beta(y)}{\delta\bar{q}_\alpha(x)} = \delta_{\alpha\beta}\delta^4(x-y) - \eta(y)\Gamma_{\alpha\beta}\delta^4(x-y) + \mathcal{O}(\eta^2). \tag{A34}$$

Using the identity

$$\mathrm{Det}\, M = \exp\mathrm{Tr}\ln M, \tag{A35}$$

we readily obtain the Jacobian as

$$\mathrm{Det}\left\{\frac{\delta\bar{q}'}{\delta\bar{q}}\right\} = \exp\left[-\mathrm{Tr}(\Gamma)\int d^4x\eta(x)\delta^4(x-x)\right]. \tag{A36}$$

It is found that if the trace of the matrix Γ is nonzero, the Jacobian yields a singular factor, while if it vanishes, we need careful treatment for evaluating this term. So, in the following discussion, we divide Γ into two types; one is the term proportional to the unit matrix, and the other is the traceless part.

First, we consider the case $\Gamma \propto \mathbb{1}$. Using Eqs. (A31), (A33), and (A36), we obtain the following equation:

$$\langle 0|\bar{q}\Gamma(i\not{D} - m_q)q|0\rangle_\theta = -i\mathrm{Tr}(\Gamma)\delta^4(0). \tag{A37}$$

Once we carry out the normal ordering for the composite operator $\bar{q}\Gamma(i\not{D} - m_q)q$, the singular factor in the right-hand side vanishes. Thus we conclude that, after normal ordering,

$$\langle 0|\bar{q}\Gamma(i\not{D} - m_q)q|0\rangle_\theta = 0, \tag{A38}$$

when $\Gamma \propto \mathbb{1}$. This equation implies that we may use the equations of motion for quark condensates in this case.

Next, we shall turn to the traceless part. In this case, the Jacobian in Eq. (A36) is written in terms of the anomaly function defined as

$$\mathcal{A}(x) \equiv 2\mathrm{Tr}(\Gamma)\delta^4(x-x). \tag{A39}$$

With this function, Eq. (A36) leads to

$$\mathrm{Det}^{-1}\left\{\frac{\delta\bar{q}'}{\delta\bar{q}}\right\} = \exp\left[+\frac{1}{2}\int d^4x\eta(x)\mathcal{A}(x)\right]. \tag{A40}$$

The usual analysis for the chiral anomaly tells us that the function $\mathcal{A}(x)$ in Eq. (A39) does not vanish only for the case $\Gamma = \gamma_5$. Thus, if $\Gamma \neq \gamma_5$, Eq. (A38) is satisfied. When $\Gamma = \gamma_5$, on the other hand, the function $\mathcal{A}(x)$ is evaluated as

$$\mathcal{A}(x) = \frac{\alpha_s}{4\pi}G^A_{\mu\nu}\tilde{G}^{A\mu\nu}. \tag{A41}$$

From Eqs. (A31), (A33), and (A40), we eventually find that

$$\langle 0|\bar{q}\gamma_5(i\not{D} - m_q)q|0\rangle_\theta = -\frac{i\alpha_s}{8\pi}\langle 0|G^A_{\mu\nu}\tilde{G}^{A\mu\nu}|0\rangle_\theta. \tag{A42}$$

This expression is simplified via the axial current anomaly equation:

$$\partial^\mu(\bar{q}\gamma_\mu\gamma_5 q) = 2im_q\bar{q}\gamma_5 q + \frac{\alpha_s}{4\pi}G^A_{\mu\nu}\tilde{G}^{A\mu\nu}. \tag{A43}$$

Then, Eq. (A42) leads to

$$\langle 0|\bar{q}\gamma_5 i\not{D}q|0\rangle_\theta = \frac{1}{2i}\langle 0|\partial^\mu(\bar{q}\gamma_\mu\gamma_5 q)|0\rangle_\theta = 0. \tag{A44}$$

Therefore, we are not able to use the classical equations of motion for quark condensates in this case.

As a result, we find that

$$\langle 0|\bar{q}\Gamma i\not{D}q|0\rangle_\theta = \begin{cases}\langle 0|\bar{q}\Gamma m_q q|0\rangle_\theta & (\text{for } \Gamma = \mathbb{1}, \gamma_\mu, \gamma_\mu\gamma_5, \sigma_{\mu\nu})\\ 0 & (\text{for } \Gamma = \gamma_5).\end{cases} \tag{A45}$$

Also, its conjugate leads to

$$-\langle 0|\bar{q}i\overleftarrow{\not{D}}\Gamma q|0\rangle_\theta = \begin{cases}\langle 0|\bar{q}m_q\Gamma q|0\rangle_\theta & (\text{for } \Gamma = \mathbb{1}, \gamma_\mu, \gamma_\mu\gamma_5, \sigma_{\mu\nu})\\ 0 & (\text{for } \Gamma = \gamma_5).\end{cases} \tag{A46}$$

Before concluding the section, we add a comment on the condensate of the total derivative terms. As we have already conducted in Eq. (A44), the Lorentz invariance of vacuum implies that condensates of the divergence of quark bilinear always vanish, i.e.,

$$\langle 0|\partial^\mu(\bar{q}\Gamma_\mu q)|0\rangle = \partial^\mu\langle 0|(\bar{q}\Gamma_\mu q)|0\rangle = 0, \tag{A47}$$

with Γ_μ a constant matrix which transforms as a vector under the Lorentz transformation, such as γ_μ, $\gamma_\mu\gamma_5$, or so on. On the other hand, the total derivative of the quark bilinear is written as

$$\partial^\mu(\bar{q}\Gamma_\mu q) = (\partial^\mu \bar{q})\Gamma_\mu q + \bar{q}\Gamma_\mu(\partial^\mu q) = \bar{q}\overleftarrow{D}^\mu \Gamma_\mu q + \bar{q}\Gamma_\mu D^\mu q. \tag{A48}$$

Thus we find

$$\langle 0|\bar{q}\overleftarrow{D}^\mu \Gamma_\mu q|0\rangle = -\langle \bar{q}\Gamma_\mu D^\mu q|0\rangle. \tag{A49}$$

3. WILSON LINE IN FOCK-SCHWINGER GAUGE

Quark fields $q(x)$ are always accompanied by an appropriate Wilson-line operator in order to compensate the different gauge transformation property of the quark fields at different space-time points. In the Fock-Schwinger gauge, however, one may always choose a particular path which makes the Wilson-line operator equal to identity [32]. We show this statement in the following. The Wilson line is written as

$$U_P(x,0) = P\left\{\exp\left[ig_s\int_0^1 ds\frac{dx'^\mu(s)}{ds}G_\mu^A(x'(s))T^A\right]\right\}, \tag{A50}$$

where

$$x'(0) = 0, \qquad x'(1) = x, \tag{A51}$$

and P denotes path ordering. This operator depends on the choice of the integration path. Here we take a path such that

$$x'(s) = sx. \tag{A52}$$

Then,

$$U_P(x,0) = P\left\{\exp\left[ig_s\int_0^1 dsx^\mu G_\mu^A(sx)T^A\right]\right\}. \tag{A53}$$

In the Fock-Schwinger field, the gluon field is expanded as

$$G_\mu(x) = \frac{1}{2\cdot 0!}x^\nu G_{\nu\mu}(0) + \frac{1}{3\cdot 1!}x^\alpha x^\nu(D_\alpha G_{\nu\mu}(0)) + \frac{1}{4\cdot 2!}x^\alpha x^\beta x^\nu(D_\alpha D_\beta G_{\nu\mu}(0)) + \cdots. \tag{A54}$$

Inserting this expression into Eq. (A53), we readily find that all terms in the exponential vanish due to the antisymmetric property of the gluon field strength tensor. Therefore,

$$U_P(x,0) = 1. \tag{A55}$$

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