Chiral perturbation theory in a θ vacuum

著者	Aoki Sinya, Fukaya Hidenori
journal or publication title	Physical review D
volume	81
number	3
page range	034022
year	2010-02
権利	(C) 2010 The American Physical Society
URL	http://hdl.handle.net/2241/104863

PHYSICAL REVIEW D **81,** 034022 (2010)

Chiral perturbation theory in a θ vacuum

Sinya Aoki[1,2] and Hidenori Fukaya[3]

[1]*Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan*
[2]*Riken BNL Research Center, Brookhaven National Laboratory, Upton, New York 11973, USA*
[3]*Department of Physics, Nagoya University, Nagoya 464-8602, Japan*
(Received 12 July 2009; published 16 February 2010)

We consider chiral perturbation theory with a nonzero θ term. Because of the CP violating term, the vacuum of chiral fields is shifted to a nontrivial element on the $SU(N_f)$ group manifold. The CP violation also provides mixing of different CP eigenstates, between scalar and pseudoscalar, or vector and axialvector, operators. We investigate up to $\mathcal{O}(\theta^2)$ effects on the mesonic two-point correlators of chiral perturbation theory to the one-loop order. We also address the effects of fixing topology, by using saddle-point integration in the Fourier transform with respect to θ.

DOI: 10.1103/PhysRevD.81.034022 PACS numbers: 12.39.Fe, 12.38.Gc

I. INTRODUCTION

The low energy limit of quantum chromo dynamics (QCD) is full of nonperturbative phenomena such as quark confinement and chiral symmetry breaking. It has, however, been very difficult to analytically investigate these phenomena from the first principle due to its nonlinearity and strong coupling of interactions. Lattice QCD [1] and chiral perturbation theory (ChPT) [2,3] have played prominent roles in studying such dynamical phenomena of QCD. The nonperturbative calculations of lattice QCD can be numerically performed utilizing the latest computational resources, while ChPT, an effective theory of pions, allows us to perturbatively treat the very low energy limit of QCD. They are complementary each other and have mutually developed. Lattice QCD in principle can determine the low energy constants of ChPT, some of which are difficult to determine from experimental inputs. On the other hand, ChPT provides a theoretical guideline of how to extrapolate the lattice data to the near-zero quark mass limit (chiral extrapolation) or the infinite volume limit (finite size scaling).

An interesting extension of QCD is to introduce a CP violation term, known as the θ term. Since it is written as a total derivative in the QCD Lagrangian, it exists only when the gauge fields can have a nontrivial topological structure, or winding numbers. By partial integration, this θ term can be regarded as the phase of superposition of different vacua in the Hamilton picture, which we call the θ vacuum [4].

CP is invariant non only at $\theta = 0$ but also at $\theta = \pi$. It is, however, believed that CP is spontaneously broken at $\theta = \pi$, where the theory has two CP violating vacua [5]. Moreover, it is expected that there exists a first-order phase transition in $0 < \theta \leq \pi$. These issues have been investigated mainly using some effective theories [6].

It is little known in nature why this CP violation term is invisibly suppressed, which is the so-called strong CP problem. The neutron electric dipole moment has not been observed in the experiments, from which one can estimate $|\theta| \lesssim 10^{-10}$ [7]. The lattice QCD community has also tried to *quantify* the strong CP problem [8]. It remains, however, to be one of the most difficult problems in lattice QCD, since the θ term gives a complex action, which leads to the notorious phase problem in Monte-Carlo simulations. With various elaborated approaches, many groups have investigated the θ vacuum in the lattice simulations [9,10].

There exists another motivation in studying the θ vacuum of QCD. One can consider a fixed topological sector of the theory, by Fourier transform of the partition function with respect to θ. Expanding the vacuum energy as $f(\theta) = c_2\theta^2/2 + c_4\theta^4/4! \cdots$ and performing the saddle-point integration order by order, one can investigate how the topology affects the physical quantities and evaluate the difference between the physics between the θ vacuum and the one at fixed topology [11,12]. Inversely, it is also possible to determine the vacuum energy of QCD as a power series of θ, from the physical observables at fixed topology. In Refs. [11,12], a general formula to $\mathcal{O}(1/V^2)$ is calculated which converts the observables at fixed topology to those in $\theta = 0$ vacuum treating $c_2, c_4, \cdots$ as unknown parameters. It is, therefore, an important task to calculate these parameters within QCD or the low energy effective theory to quantify the effects of fixing topology.

In fact, QCD at fixed topology can be investigated by lattice QCD simulations. Employing the overlap Dirac operator [13], which preserves the exact chiral symmetry, we are able to define the topological charge on the lattice. JLQCD and TWQCD Collaborations are using a topology preserving way [14] to avoid discontinuities of the overlap fermion determinant, which considerably reduces the computational cost. The conversion formula between θ vacuum and fixed topology is, therefore, essential in extracting the low energy constants such as the chiral condensate Σ [15], the pion decay constant F [16], and the topological susceptibility [17].

Because of its *global* topological nature, the θ vacuum effect is totally infrared physics and, therefore, should be described by the lightest particles, or pions, within chiral perturbation theory. In this paper, we discuss ChPT with nonzero value of θ as well as at a fixed topology. The formulation and general qualitative discussion are already given in Refs. [3,18]. Our goal is to explicitly calculate the meson correlators to the next-leading order (NLO) in the θ vacuum (and in a fixed topological sector) at finite volume, which may be directly compared with lattice QCD. In Sec. II, we will observe that the vacuum of chiral fields is located not at identity but at a nontrivial element on the $SU(N_f)$ group manifold. In the p expansion of the chiral Lagrangian, this vacuum shift provides as a source which mixes the different CP eigenstates (Sec. III). In Sec. IV, we will calculate the θ vacuum effect upto $\mathcal{O}(\theta^2)$ on the mesonic two-point correlation functions in ChPT to the next-to-leading order. In Sec. V, we will also address the physics at fixing topology, by using the saddle-point integration in the Fourier transform with respect to θ, as discussed above. The concluding remarks are given in Sec. VI.

II. CHIRAL LAGRANGIAN TO THE LEADING ORDER

We consider the N_f-flavor chiral Lagrangian in the θ vacuum,

$$\mathcal{L} = \frac{F^2}{4}\mathrm{Tr}[\partial_\mu U(x)^\dagger \partial_\mu U(x)] - \frac{\Sigma}{2}\mathrm{Tr}[\mathcal{M}^\dagger e^{-i\theta/N_f}U(x) + U(x)^\dagger e^{i\theta/N_f}\mathcal{M}] + \cdots, \tag{1}$$

where $U(x) \in SU(N_f)$, Σ is the chiral condensate, and F denotes the pion decay constant both in the chiral limit. Here θ, the QCD vacuum angle, appears as the phase of the mass term, reflecting the picture that the θ term can be converted to the chiral rotation of the quark bilinears through the anomalous Ward-Takahashi identity. In the mass matrix,

$$\mathcal{M} = \mathrm{diag}(\underbrace{m_v, m_{v'}, \cdots}_{N_v}, \underbrace{m_1, m_2, \cdots}_{N_f}), \tag{2}$$

we have N_v valence flavors and N_f dynamical flavors.

In the partially quenched case [19], we use the so-called replica trick, where the calculations are done with $[N_f + N_v + (N - N_v)]$-flavor theory and then the replica limit $N \to 0$ is taken. The full theory results are precisely obtained by choosing $m_v = m_f$, where m_f denotes one of the dynamical quark masses.

The system is assumed to be in the so-called p regime, where the Euclidean space-time volume $V = L^3T$ is large enough so that the perturbative expansion is performed according to the counting rule,

$$\partial_\mu \sim \mathcal{O}(p), \qquad \xi(x) \sim \mathcal{O}(p), \qquad \mathcal{M} \sim \mathcal{O}(p^2), \qquad T, L \sim \mathcal{O}(1/p), \tag{3}$$

in the units of a cutoff scale.

Note that due to the vacuum angle θ, the expectation value of $U(x)$ is located not at the identity but a nontrivial element of $SU(N_f)$ (let us denote U_0). It is, therefore, useful to define the new variable and mass matrix,

$$U(x) \equiv U_0\tilde{U}(x), \qquad \mathcal{M}_\theta \equiv U_0^\dagger e^{i\theta/N_f}\mathcal{M}, \tag{4}$$

and rewrite the Lagrangian,

$$\mathcal{L} = \frac{F^2}{4}\mathrm{Tr}[\partial_\mu \tilde{U}(x)^\dagger \partial_\mu \tilde{U}(x)] - \frac{\Sigma}{2}\mathrm{Tr}[\mathcal{M}_\theta^\dagger \tilde{U}(x) + \tilde{U}(x)^\dagger \mathcal{M}_\theta] + \cdots, \tag{5}$$

where $\tilde{U}(x)$ can be expanded around the identity as usual;

$$\tilde{U}(x) = \exp\left(i\frac{\sqrt{2}\xi(x)}{F}\right) \sim 1 + i\frac{\sqrt{2}\xi(x)}{F} - \frac{\xi^2(x)}{F^2} - \frac{i\sqrt{2}\xi^3(x)}{3F^3} + \frac{\xi^4(x)}{6F^4} + \cdots, \tag{6}$$

where ξ is an element of $SU(N_f)$ Lie algebra.

By this vacuum shift, Eq. (5) explicitly shows that the nonzero θ vacuum physics is equivalent to that in the $\theta = 0$ vacuum but with a complex mass matrix $\mathcal{M}_\theta$. Our task in the following is, therefore, to determine U_0 (or equivalently $\mathcal{M}_\theta$) and then to calculate the difference between the systems with the complex $\mathcal{M}_\theta$ and a simply real diagonal $\mathcal{M}$.

A. Vacuum shift U_0

Let us first calculate the vacuum expectation value U_0, which minimizes the Lagrangian density of the zero-mode

$$\mathcal{L}_0 = -\frac{\Sigma}{2}\mathrm{Tr}[\mathcal{M}^\dagger e^{-i\theta/N_f}U_0 + U_0^\dagger e^{i\theta/N_f}\mathcal{M}]. \tag{7}$$

For small θ, by parametrizing $U_0 = \exp(i\xi^0)$, the problem is equivalent to finding the minimum of a potential

$$V(\xi^0) = \sum_i^{N_f} m_i\left[-\sin\left(\frac{\theta}{N_f}\right)\left[\xi^0 - \frac{1}{6}(\xi^0)^3\right]_{ii} + \frac{1}{2}\cos\left(\frac{\theta}{N_f}\right)\left[(\xi^0)^2 - \frac{1}{12}(\xi^0)^4\right]_{ii}\right] + \lambda\,\mathrm{Tr}[\xi^0], \tag{8}$$

where λ denotes the Lagrange's multiplier to guarantee the traceless solution.

It can be recursively shown, order by order, that all the off-diagonal parts of ξ^0 are zero. For the diagonal elements, one obtains

$$\xi^0_{ii} = \bar{\theta} - \frac{\bar{m}}{m_i}\theta + a_i\theta^3 + \mathcal{O}(\theta^5), \tag{9}$$

where

$$\bar{\theta} \equiv \frac{\theta}{N_f}, \qquad \bar{m} \equiv \frac{1}{\sum_f^{N_f} 1/m_f},$$
$$a_i \equiv \frac{\bar{m}^3}{6}\left(\frac{\bar{m}}{m_i}\sum_f^{N_f}\frac{1}{m_f^3} - \frac{1}{m_i^3}\right). \tag{10}$$

Note that the partially quenched result is obtained simply by taking $m_i = m_v$ after the replica limit. It is also notable that $\xi_{ii}^0 = 0$ when m_i's are all degenerate.

Now the original Lagrangian in Eq. (7) is greatly simplified;

$$\mathcal{L}_0 = -\Sigma\left[\sum_f^{N_f} m_f \cos\left(\frac{\bar{m}}{m_f}\theta - a_f\theta^3\right)\right], \tag{11}$$

from which one can read off the vacuum energy density at the tree level,[1] as a function of θ. In particular, the coefficients of θ^2 (the topological susceptibility χ_t) and θ^4 (we denote c_4),

$$\chi_t = \frac{d^2\mathcal{L}_0}{d\theta^2}\bigg|_{\theta=0} = \bar{m}\Sigma, \tag{12}$$

$$c_4 = \frac{d^4\mathcal{L}_0}{d\theta^4}\bigg|_{\theta=0} = -\bar{m}\Sigma\left(\sum_f^{N_f}\frac{\bar{m}^3}{m_f^3}\right), \tag{13}$$

are important when we consider the effect of fixing topology as previously discussed in Refs. [11,12].

Another important observation follows from the fact

$$\mathrm{Im}\,(\mathcal{M}_\theta) = \bar{m}\theta\mathbf{1} + \mathcal{O}(\theta^3), \tag{14}$$

where $\mathbf{1}$ denotes the $N_f \times N_f$ identity matrix. Noting $\mathrm{Tr}\xi = 0$, the contribution from the imaginary part of the mass matrix then becomes $\sim\mathcal{O}(p^5)$ so that we can neglect it at the leading order.[2]

In this subsection, we have derived the vacuum expectation value U_0 upto $\mathcal{O}(\theta^4)$ level. The most part of this paper, however, requires only $\mathcal{O}(\theta^2)$ contribution and one can neglect the 3rd term of Eq. (9) or set $a_i = 0$.

B. Propagator of $\xi(x)$

Let us now expand the Lagrangian in ξ,

$$\mathcal{L} = \mathcal{L}_0 + \frac{1}{2}\sum_{i,j}^{N_f}[\xi(x)]_{ij}(-\partial_\mu^2 + M_{ij}^2(\theta))[\xi(x)]_{ji} + \cdots. \tag{15}$$

Here, $M_{ij}^2(\theta)$ is given by

$$M_{ij}^2(\theta) = \frac{\Sigma}{F^2}(m_i(\theta) + m_j(\theta)), \tag{16}$$

where $m_i(\theta)$ is defined by

$$m_i(\theta) = m_i\cos\left(\frac{\bar{m}}{m_i}\theta - a_i\theta^3\right)$$
$$= m_i\left(1 - \frac{1}{2}\frac{\bar{m}^2}{m_i^2}\theta^2\right) + \mathcal{O}(\theta^4), \tag{17}$$

and again there is no significant difference even if we extend the theory to the partially quenched one; we just set $m_i = m_v$.

The Feynmann propagator (in a finite volume) is then obtained:

$$\langle\xi_{ij}(x)\xi_{kl}(y)\rangle_\xi = \delta_{il}\delta_{jk}\Delta(x-y, M_{ij}^2(\theta)) - \delta_{ij}\delta_{kl}G(x-y, M_{ii}^2(\theta), M_{kk}^2(\theta)), \tag{18}$$

where the second term comes from the traceless constraint $\mathrm{Tr}\xi = 0$. The definitions of Δ and G are given by (unless $N_f = 0$)

$$\Delta(x, M^2) = \frac{1}{V}\sum_p \frac{e^{ipx}}{p^2 + M^2}, \tag{19}$$

$$G(x, M_{ii}^2, M_{jj}^2) = \frac{1}{V}\sum_p \frac{e^{ipx}}{(p^2 + M_{ii}^2)(p^2 + M_{jj}^2)(\sum_f^{N_f}\frac{1}{p^2 + M_{ff}^2(\theta)})}, \tag{20}$$

where the summation is taken over the 4-momentum

$$p = 2\pi(n_t/T, n_x/L, n_y/L, n_z/L), \tag{21}$$

with integers n_i's.

III. ONE-LOOP CORRECTIONS

Since we are interested in at most one-loop corrections to the two-point functions, we can take, in advance, some Wick contractions in $\mathcal{O}(p^5)$ or $\mathcal{O}(p^6)$ contributions in the expansion of the leading order Lagrangian Eq. (15).

Before performing the one-loop calculation, we here introduce the NLO terms of the chiral Lagrangian. Without source terms, we have 8 additional NLO terms whose low energy constants are denoted by L_i's ($i = 1\cdots 8$).[3] At $\mathcal{O}(p^5)$ and $\mathcal{O}(p^6)$, the terms with L_1, L_2, L_3 (and Wess-Zunimo-Witten term [22]) do not contribute to our calculation. For the terms with L_4, L_5, L_6, the NLO correction is obtained in the same way as the $\theta = 0$ case except for the change in the mass matrix; $\mathcal{M} \to \mathrm{Re}\mathcal{M}_\theta$, while the L_7 and L_8 terms require a special care of the imaginary part of the mass matrix, $\mathrm{Im}\mathcal{M}_\theta = \bar{m}\theta\mathbf{1}$.

[1] For the $N_f = 2$ case, a nonperturbative expression of the vacuum energy density is known [20], from which one can read off χ_t, c_4 [21], and any higher order coefficients c_{2n}'s.
[2] It of course gives contributions at NLO.

[3] When $N_f = 2$, due to the pseudoreality, the number of independent terms is reduced to 5, of which coefficients are denoted by l_i's [3].

Expanding the chiral field according to Eq. (6), we obtain

$$\mathcal{L}_{\rm NLO} = \sum_{i,j}\left[\frac{1}{2}\partial_\mu\xi_{ij}\partial_\mu\xi_{ji}\right]\times\frac{8}{F^2}\left[L_4\sum_f M_{ff}^2(\theta)+L_5M_{ij}^2(\theta)\right]+\sum_{i,j}\left[\frac{1}{2}\xi_{ij}\xi_{ji}\right]\times M_{ij}^2(\theta)\frac{16}{F^2}L_6\sum_f M_{ff}^2(\theta)$$
$$+\frac{8L_7}{F^2}\sum_{i,j}^{N_f}M_{ii}^2(\theta)M_{jj}^2(\theta)\xi_{ii}\xi_{jj}+\frac{1}{2}\sum_{i,j}\xi_{ij}\xi_{ji}\frac{16L_8}{F^2}M_{ij}^4(\theta)-\frac{8\sqrt{2}(N_fL_7+L_8)\bar{M}^2\theta}{F}\sum_i^{N_f}M_{ii}^2(\theta)\xi_{ii}$$
$$-\frac{16(N_fL_7+L_8)}{F^2}(\bar{M}^4\theta^2)\sum_{i,j}^{N_f}\frac{1}{2}\xi_{ij}\xi_{ji},-4L_6\left(\sum_f M_{ff}^2(\theta)\right)^2-2L_8\sum_f M_{ff}^4(\theta=0)+4N_f(N_fL_7+L_8)\bar{M}^4\theta^2$$
$$+\mathcal{O}(p^7), \tag{22}$$

where $\bar{M}^2 = 2\bar{m}\Sigma/F^2$ and we have used $[(\mathrm{Re}\mathcal{M}_\theta)^2]_{ii} = [(\mathcal{M}_{\theta=0})^2 - (\mathrm{Im}\mathcal{M}_\theta)^2]_{ii} + \mathcal{O}(\theta^3)$. The first 4 terms can be absorbed into the redefinition of kinetic and mass terms, as usual in the case with $\theta = 0$. The 5th and 6th terms represent a peculiar contribution due to nonzero θ. We have kept the constant (but θ dependent) terms in the last 3 terms for the calculation of topological susceptibility, which we will address later.

A. Vacuum shift at one-loop

Let us start with $\mathcal{O}(p^5)$ terms, which appears only in the nonzero θ vacuum:

$$\mathcal{L}_5 = \theta\left[\frac{\sqrt{2}}{6F}\bar{M}^2\,\mathrm{Tr}\xi^3 - \frac{\sqrt{2}}{2F}\bar{M}^2\sum_i^{N_f}(16(N_fL_7+L_8)\times M_{ii}^2(\theta)\xi_{ii})\right]. \tag{23}$$

Taking contractions of ξ's in the first term, and noting $\sum_i\xi_{ii} = 0$, it becomes

$$\mathcal{L}_5 \to \theta\left[\sum_i\frac{F}{\sqrt{2}}M_{ii}^2B_{ii}\xi_{ii}(x)\right]+\mathcal{O}(\theta^3), \tag{24}$$

where

$$B_{ii} \equiv \frac{\bar{m}}{m_i}\times\frac{1}{F^2}\Bigg[\Bigg(\sum_f^{N_f}\Delta(0,M_{if}^2) - G(0,M_{ii}^2,M_{ii}^2) - 16(N_fL_7+L_8)M_{ii}^2\Bigg) - \frac{1}{N_f}\sum_j^{N_f}\Bigg(\sum_f^{N_f}\Delta(0,M_{jf}^2) - G(0,M_{jj}^2,M_{jj}^2) - 16(N_fL_7+L_8)M_{jj}^2\Bigg)\Bigg], \tag{25}$$

which gives an $\mathcal{O}(p^2)$ contribution. Here, θ dependence of the masses is dropped, since it gives only $\mathcal{O}(\theta^3)\times\mathcal{O}(p^2)$ contributions; we have simply set $M_{ij}^2 = M_{ij}^2(\theta=0)$ in (25). Note also that $\sum_i M_{ii}^2B_{ii} = 0$.

The above linear term in ξ in Eq. (24) requires further shift in the vacuum $U_0(\times e^{-i\theta/N_f})$;

$$U_0e^{-i\theta/N_f} \to U_0' \equiv \mathrm{diag}(e^{-i\theta_1}, e^{-i\theta_2},\cdots), \tag{26}$$

where the phase of ith diagonal component is given by

$$\theta_i \equiv \frac{\bar{m}}{m_i}\theta - a_i\theta^3 - b_i\theta, \tag{27}$$

with

$$b_i \equiv -B_{ii} + \frac{\bar{m}}{m_i}\sum_f^{N_f}B_{ff}. \tag{28}$$

Again, we have ignored $\mathcal{O}(\theta^3)\times\mathcal{O}(p^2)$ contributions here.

The meson mass is also shifted as

$$M_{ij}^2(\theta) \to (M_{ij}'(\theta))^2 \equiv \frac{\Sigma}{F^2}(m_i\cos\theta_i + m_j\cos\theta_j), \tag{29}$$

and the effective Lagrangian up to $\mathcal{O}(p^5)$ then reads

$$\mathcal{L}_{\rm LO} + \mathcal{L}_5 = \frac{1}{2}\mathrm{Tr}(\partial_\mu\xi(x))^2 + \frac{1}{2}\sum_i^{N_f}(M_{ii}'(\theta))^2[\xi^2(x)]_{ii} + \frac{\sqrt{2}}{6F}\bar{M}^2\theta\left(\mathrm{Tr}\xi^3 - 3\sum_i^{N_f}\langle\xi_{ii}^2\rangle_\xi\xi_{ii}\right). \tag{30}$$

B. Inserting sources

Next, we consider insertions of the pseudoscalar and axial vector sources, $p(x)$ and $a_\mu(x)$. Since the parity symmetry is broken by the θ term, we will see that these source terms have unusual contributions which look like scalar or vector operators. It is therefore convenient to define the *shifted* Hermitian sources as

$$p^+(x) \equiv \tfrac{1}{2}(U_0'^\dagger p(x) + p(x)U_0'), \tag{31}$$

$$p^-(x) \equiv \frac{i}{2}(U_0'^\dagger p(x) - p(x)U_0'), \tag{32}$$

$$a_\mu^+(x) \equiv \tfrac{1}{2}(U_0'^\dagger a_\mu(x)U_0' + a_\mu(x)), \tag{33}$$

$$a_\mu^-(x) \equiv \frac{i}{2}(U_0'^\dagger a_\mu(x)U_0' - a_\mu(x)), \tag{34}$$

where we have assumed the original $p(x)$ and $a_\mu(x)$ are both Hermitian and traceless matrices. In the following, we consider only charged meson type sources which have two different flavor indices. For this case the absence of the diagonal parts: $[p]_{ii} = [p^+]_{ii} = [p^-]_{ii} = 0$ and $[a_\mu]_{ii} = [a^+_\mu]_{ii} = [a^-_\mu]_{ii} = 0$ (for all i) simplifies the calculation.

C. One-loop effective Lagrangian with sources

In the expansion of the leading Lagrangian Eq. (15), we also have $\mathcal{O}(p^6)$ terms,

$$\frac{1}{6F^2}\,\mathrm{Tr}[\partial_\mu\xi\xi\partial_\mu\xi\xi - \xi^2(\partial_\mu\xi)^2] - \frac{1}{12F^2}\sum_i^{N_f} M^2_{ii}(\theta)[\xi^4]_{ii}, \tag{35}$$

from which contribution can be calculated in a straightforward way as in the case at $\theta = 0$ [3].

Collecting all contributions so far, the LO + NLO effective Lagrangian, including the pseudoscalar and axial vector sources, is given by

$$\begin{aligned}\mathcal{L}^\theta_{\mathrm{eff}}(p, a_\mu) &= \frac{1}{2}\sum_{i,j}^{N_f}(Z^{ij}_\xi(\theta))^2([\partial_\mu\xi_{ij}\partial_\mu\xi_{ji}](x) + (M'_{ij}(\theta))^2(Z^{ij}_M(\theta))^2[\xi_{ij}\xi_{ji}](x)) + \frac{\sqrt{2}}{6F}\bar{M}^2\theta\Big(\mathrm{Tr}\xi^3(x) - 3\sum_i^{N_f}\langle\xi^2_{ii}\rangle_\xi\xi_{ii}(x)\Big)\\
&+ \frac{1}{2}\sum_{i,j}^{N_f}[\xi_{ij}\xi_{ji}(x)]\times\Big(-\frac{16}{F^2}(N_f L_7 + L_8)\bar{M}^4\theta^2\Big) - \frac{\sqrt{2}\Sigma}{F}\sum_{i,j}^{N_f}[p^+_{ji}(x)\xi_{ij}(x)]\times Z^{ij}_\xi(\theta)Z^{ij}_F(\theta)(Z^{ij}_M(\theta))^2\\
&+ \sum_{i,j}^{N_f}\Big[p^-_{ji}(x)\Big(\frac{\Sigma}{F^2}\xi^2_{ij}(x) - \frac{16\sqrt{2}\Sigma(N_f L_7 + L_8)}{F^3}\bar{M}^2\theta\xi_{ij}(x)\Big)\Big] - \sqrt{2}F\sum_{i,j}^{N_f}[a^+_\mu(x)_{ji}\partial_\mu\xi_{ij}(x)]\times Z^{ij}_\xi(\theta)Z^{ij}_F(\theta)\\
&+ \sum_{i,j}^{N_f}[a^-_\mu(x)]_{ji}[\partial_\mu\xi(x)\xi(x) - \xi(x)\partial_\mu\xi(x)]_{ij} + \frac{1}{2F^2}\sum_{i,j}^{N_f}\Big([\partial_\mu\xi_{ii}\partial_\mu\xi_{jj}](x)\frac{\Delta(0, M^2_{ij}(\theta))}{3}\\
&- \Big(\frac{2}{3}M^2_{ij}(\theta)\Delta(0, M^2_{ij}(\theta)) - 16L_7 M^2_{ii}(\theta)M^2_{jj}(\theta)\Big)[\xi_{ii}\xi_{jj}](x)\Big) - \Sigma\Big(\sum_f^{N_f} m_f\cos\theta_f\Big) - 4L_6\Big(\sum_f M^2_{ff}(\theta)\Big)^2\\
&+ 4N_f(N_f L_7 + L_8)\bar{M}^4\theta^2,\end{aligned} \tag{36}$$

where we have omitted θ-independent constants. We also have omitted multi n point vertices for $n > 3$, which are irrelevant for the two-point correlation functions below.

In the above result, the Z factors are given by

$$Z^{ij}_\xi(\theta) \equiv 1 - \frac{1}{2F^2}\Big[\frac{\sum_f^{N_f}(\Delta(0, M^2_{if}(\theta)) + \Delta(0, M^2_{jf}(\theta)))}{6} + \frac{A(0, M^2_{ii}(\theta), M^2_{jj}(\theta))}{3} - 8\Big(L_4\sum_f^{N_f} M^2_{ff}(\theta) + L_5 M^2_{ij}(\theta)\Big)\Big], \tag{37}$$

$$Z^{ij}_M(\theta) \equiv 1 + \frac{1}{2F^2}\Big[G(0, M^2_{ii}(\theta), M^2_{jj}(\theta)) - 8(L_4 - 2L_6)\sum_f^{N_f} M^2_{ff}(\theta) - 8(L_5 - 2L_8)M^2_{ij}(\theta)\Big], \tag{38}$$

$$Z^{ij}_F(\theta) \equiv 1 - \frac{1}{2F^2}\Big[\frac{\sum_f^{N_f}(\Delta(0, M^2_{if}(\theta)) + \Delta(0, M^2_{jf}(\theta)))}{2} + A(0, M^2_{ii}(\theta), M^2_{jj}(\theta)) - 8\Big(L_4\sum_f^{N_f} M^2_{ff}(\theta) + L_5 M^2_{ij}(\theta)\Big)\Big], \tag{39}$$

where

$$A(x, M^2_{ii}, M^2_{jj}) \equiv G(x, M^2_{ii}, M^2_{jj}) - \frac{G(x, M^2_{ii}, M^2_{ii}) + G(x, M^2_{jj}, M^2_{jj})}{2} \tag{40}$$

and its derivative

$$\partial_\mu^2 A(x, M_{ii}^2, M_{jj}^2) = M_{ij}^2 G(x, M_{ii}^2, M_{jj}^2) - \frac{M_{ii}^2 G(x, M_{ii}^2, M_{ii}^2) + M_{jj}^2 G(x, M_{jj}^2, M_{jj}^2)}{2} \tag{41}$$

are UV finite at $x = 0$, and both vanish when $M_{jj}^2 = M_{ii}^2$.

On the other hand, $\Delta(0, M^2)$ and $G(0, M_1^2, M_2^2)$ are logarithmically divergent, and the divergent parts are evaluated by the dimensional regularization at $D = 4 - 2\epsilon$ as

$$\Delta(0, M^2) = -\frac{M^2}{16\pi^2}\left(\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi\right) + \cdots,$$

$$G(0, M_1^2, M_2^2) = -\frac{1}{16\pi^2}\left(\frac{M_1^2 + M_2^2}{N_f} - \frac{1}{N_f^2}\sum_f^{N_f} M_{ff}^2(\theta)\right) \times \left(\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi\right) + \cdots, \tag{42}$$

where $\gamma = 0.57721\cdots$ denotes Euler's constant. As is the usual case, these divergence can be removed by the renormalization of L_i's as

$$L_i = L_i^r(\mu_{\rm sub}) - \frac{\gamma_i}{32\pi^2}\left(\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi - \ln \mu_{\rm sub}^2\right), \tag{43}$$

where $L_i^r(\mu_{\rm sub})$'s denote the renormalized low energy constants at the subtraction scale $\mu_{\rm sub}$, and

$$\gamma_4 = \frac{1}{8}, \qquad \gamma_5 = \frac{N_f}{8}, \qquad \gamma_6 = \frac{1}{8}\left(\frac{1}{2} + \frac{1}{N_f^2}\right), \qquad \gamma_7 = 0, \qquad \gamma_8 = \frac{1}{8}\left(\frac{N_f}{2} - \frac{2}{N_f}\right). \tag{44}$$

As a result, $Z_F^{ij}(\theta)$, $Z_M^{ij}(\theta)$, and $M'_{ij}(\theta)$ are kept finite, while $Z_\xi^{ij}(\theta)$ is still divergent but it does not affect the physical observables.

After this procedure, one can replace $\Delta(0, M^2)$ by

$$\Delta^r(0, M^2, \mu_{\rm sub}^2) = \frac{M^2}{16\pi^2}\ln\frac{M^2}{\mu_{\rm sub}^2} + g_1(M^2), \tag{45}$$

where g_1 denotes the finite volume contribution [23]:

$$g_1(M^2) = \sum_{a\neq 0}\int \frac{d^4q}{(2\pi)^4}\frac{e^{-iqa}}{q^2 + M^2} = \sum_{a\neq 0}\frac{M}{4\pi^2|a|}K_1(M|a|), \tag{46}$$

where K_1 is the modified Bessel function and the summation is taken over the four-vector $a_\mu = n_\mu L_\mu$ with $L_i = L$ ($i = 1, 2, 3$) and $L_4 = T$. Numerically, truncation at $|n_\mu| \leq 5$ already gives a good accuracy when $ML > 3$. For the explicit expression of $G(0, M_1^2, M_2^2)$, see Appendix A.

It is noted here that the 8th term of Eq. (36) does not contribute to the NLO two-point functions, since we consider only off-diagonal sources, $p(x)_{i\neq j}$ or $a_\mu(x)_{i\neq j}$, whose coupling to the diagonal element ξ_{ii} is of higher order [next-to-next-to-leading order (NNLO)].

IV. TWO-POINT FUNCTIONS

Pseudoscalar and axial vector correlators are obtained by the functional derivatives of the partition function

$$\mathcal{Z}^\theta(p, a_\mu) \equiv \int d\xi e^{-\int d^4x \mathcal{L}_{\rm eff}^\theta(p, a_\mu)}, \tag{47}$$

with respect to the sources p and a_μ.

Here, we derive the two-point correlation functions of these operators in an irreducible representation which consist of two different valence quarks. We consider the most general nondegenerate case where their masses are denoted by m_v and $m_{v'}$, respectively. More explicitly, we calculate the three types of correlation functions with zero momentum projection (three-dimensional integral),

$$\mathcal{P}\mathcal{P}(t, m_v, m_{v'}) \equiv \frac{1}{2}\int d^3x\left(\frac{\delta}{\delta p(x)_{vv'}} + \frac{\delta}{\delta p(x)_{v'v}}\right) \times \left(\frac{\delta}{\delta p(0)_{vv'}} + \frac{\delta}{\delta p(0)_{v'v}}\right) \times \ln \mathcal{Z}^\theta(p, a_\mu)|_{p=0, a_\mu=0}, \tag{48}$$

$$\mathcal{A}_0\mathcal{P}(t, m_v, m_{v'}) \equiv \frac{1}{2}\int d^3x\left(\frac{\delta}{\delta a_0(x)_{vv'}} + \frac{\delta}{\delta a_0(x)_{v'v}}\right) \times \left(\frac{\delta}{\delta p(x)_{vv'}} + \frac{\delta}{\delta p(0)_{v'v}}\right) \times \ln \mathcal{Z}^\theta(p, a_\mu)|_{p=0, a_\mu=0}, \tag{49}$$

$$\mathcal{A}_0\mathcal{A}_0(t, m_v, m_{v'}) \equiv \frac{1}{2}\int d^3x\left(\frac{\delta}{\delta a_0(x)_{vv'}} + \frac{\delta}{\delta a_0(x)_{v'v}}\right) \times \left(\frac{\delta}{\delta a_0(0)_{vv'}} + \frac{\delta}{\delta a_0(0)_{v'v}}\right) \times \ln \mathcal{Z}^\theta(p, a_\mu)|_{p=0, a_\mu=0}, \tag{50}$$

where we denote $t = x^0$. As mentioned before, the partial quenching is performed by the replica trick: extending the number of flavors $N_f \to N_f + N_v + (N - N_v)$ then taking the limit $N \to 0$.

Noting

$$\frac{\delta}{\delta p(x)_{vv'}} = \left(\frac{e^{i\theta_v} + e^{-i\theta_{v'}}}{2}\right)\frac{\delta}{\delta p^+(x)_{vv'}} + i\left(\frac{e^{i\theta_v} - e^{-i\theta_{v'}}}{2}\right) \times \frac{\delta}{\delta p^-(x)_{vv'}}, \tag{51}$$

$$\frac{\delta}{\delta a_\mu(x)_{vv'}} = \left(\frac{e^{i(\theta_v-\theta_{v'})}+1}{2}\right)\frac{\delta}{\delta a^+_\mu(x)_{vv'}} + i\left(\frac{e^{i(\theta_v-\theta_{v'})}-1}{2}\right)\frac{\delta}{\delta a^-_\mu(x)_{vv'}}, \quad (52)$$

the correlation functions are given by

$$\mathcal{P}\mathcal{P}(t, m_v, m_{v'}) = [C^\theta_{PP}(m_v, m_{v'})]^{\text{1-loop}} \times \frac{\cosh(M^{\text{1-loop}}_{vv'}(\theta)(t-T/2))}{M^{\text{1-loop}}_{vv'}(\theta)\sinh(M^{\text{1-loop}}_{vv'}(\theta)T/2)} + \frac{(\theta_v+\theta_{v'})^2}{4}\frac{\Sigma^2}{F^4}C^{vv'}_X(t), \quad (53)$$

$$\mathcal{A}_0\mathcal{P}(t, m_v, m_{v'}) = [C^\theta_{AP}(m_v, m_{v'})]^{\text{1-loop}} \times \frac{\sinh(M^{\text{1-loop}}_{vv'}(\theta)(t-T/2))}{\sinh(M^{\text{1-loop}}_{vv'}(\theta)T/2)} - \frac{(\theta_v^2-\theta_{v'}^2)}{4}\frac{\Sigma^2}{F^2}C^{vv'}_{Y_0}(t), \quad (54)$$

$$\mathcal{A}_0\mathcal{A}_0(t, m_v, m_{v'}) = [C^\theta_{AA}(m_v, m_{v'})]^{\text{1-loop}} M^{\text{1-loop}}_{vv'}(\theta) \times \frac{\cosh(M^{\text{1-loop}}_{vv'}(\theta)(t-T/2))}{\sinh(M^{\text{1-loop}}_{vv'}(\theta)T/2)} - \frac{(\theta_v-\theta_{v'})^2}{4}C^{vv'}_{W_{00}}(t). \quad (55)$$

Here, $[C^\theta_{JJ'}(m_v, m_{v'})]^{\text{1-loop}}$'s denote the overall coefficients of which definitions are given in Appendix C.

Because of the CP violation, each correlator has a contribution from the 2-pion state's propagation denoted by $C^{vv'}_X(t)$, $C^{vv'}_{Y_0}(t)$ and $C^{vv'}_{W_{00}}$, respectively, which are of $\mathcal{O}(e^{-2Mt})$ at large time separation (See Appendix C for the details.).

The correction to the pseudo–Nambu-Goldstone boson mass is given by

$$M^{\text{1-loop}}_{vv'}(\theta) \equiv M'_{vv'}(\theta)Z^{vv'}_M(\theta)\left(1 - \frac{\bar{M}^4\theta^2\{32(N_f L^r_7(\mu_{\text{sub}}) + L^r_8(\mu_{\text{sub}})) + H^r_{vv'}(M^2_{vv'}, \mu_{\text{sub}})\}}{4F^2M^2_{vv'}}\right), \quad (56)$$

and the pion decay constant is extracted from the $\mathcal{P}\mathcal{P}(t, m_v, m_{v'})$ and $\mathcal{A}\mathcal{P}(t, m_v, m_{v'})$ correlators in a standard way as

$$F^{\text{1-loop}}(\theta) \equiv FZ^{vv'}_F(\theta) \times \frac{Z^{vv'}_{AP}(\theta)}{\sqrt{Z^{vv'}_{PP}(\theta)}} = FZ^{vv'}_F(\theta)\left[1 - \frac{1}{8}(\theta_v-\theta_{v'})^2 - \frac{\bar{M}^4\theta^2}{4F^2}\left(\frac{\partial}{\partial M^2}H^r_{vv'}(M^2, \mu_{\text{sub}})|_{M=M_{vv'}}\right) + \frac{1}{4}(\theta_v-\theta_{v'})\frac{\bar{M}^2\theta}{F^2}H'_{vv'}(M^2_{vv'})\right]. \quad (57)$$

The definitions of $H_{ij}(M^2)$ and $H'_{ij}(M^2)$ are given in Appendix C.

One should note that for very small θ, the above formulas can be greatly simplified by ignoring $\mathcal{O}(\theta^2)\times\mathcal{O}(p^2)$ corrections or just by setting $\bar{M}^2\theta = 0$ and $M'_{vv'}(\theta) = M_{vv'}(\theta)$.

V. FIXED TOPOLOGY

From the θ dependence obtained so far, we can derive the correlators in a fixed topological sector of Q. It is known that an observable at a fixed topology (let us denote G_Q) is related to the one in the θ vacuum $[G(\theta)]$ by a formula [12],

$$G_Q = G(\theta=0) + \frac{\partial^2}{\partial\theta^2}G(\theta)|_{\theta=0}\frac{1}{2\chi_t V}\left[1 - \frac{Q^2}{\chi_t V} - \frac{c_4}{2\chi_t^2 V}\right] + \frac{\partial^4}{\partial\theta^4}G(\theta)|_{\theta=0}\frac{1}{8\chi_t^2V^2} + \mathcal{O}(V^{-3}), \quad (58)$$

which is valid in the general theories. Here, $\chi_t \equiv \langle Q^2\rangle/V$ denotes the topological susceptibility and c_4 is the coefficient of θ^4 term of the vacuum energy of the theory.

One should note that in ChPT, the θ dependence only appears in the mass term, so that we can treat $\chi_t \sim c_4 \sim \mathcal{O}(\mathcal{M}) \sim \mathcal{O}(p^2)$ in the p expansion. Therefore, the factor $1/(\chi_t V)$ reduces the order of each contribution from fixing topology by $\mathcal{O}(p^2)$, since $1/V = O(p^4)$ in the p expansion.[4] As a consequence, for nonvanishing $G(\theta=0)$, one can easily calculate the "NNLO" contribution from fixing topology with the one-loop level calculation only.

A. χ_t at one-loop

Let us first calculate χ_t within chiral perturbation theory at NLO [21]. For c_4, as explained above, the tree level calculation we have given in Eq. (13) is enough upto NNLO corrections. By switching off the source terms,

[4] In the very vicinity of the chiral limit (the ϵ-regime), $1/\chi_t V$ becomes $\mathcal{O}(1)$ and cannot be treated as peturbation. Exact integrals over θ is then needed, which is expressed by modified Bessel functions [18].

one obtains from the mass term and terms in the last line of Lagrangian Eq. (36),

$$\chi_t^{\text{1-loop}} = -\frac{1}{V}\frac{d^2}{d\theta^2}\ln Z^\theta(p=0, a_\mu=0)|_{\theta=0}$$
$$= -\Sigma\left[\sum_i^{N_f} m_i \frac{d^2}{d\theta^2}\cos\theta_i|_{\theta=0}\left(1 - \frac{\sum_j^{N_f}\langle\xi_{ij}(0)\xi_{ji}(0)\rangle_\xi^{\theta=0}}{F^2}\right)\right] - \frac{d^2}{d\theta^2}\left[4L_6\left(\sum_i^{N_f} M_{ii}^2(\theta)\right)^2 + 4N_f(N_fL_7+L_8)\bar{M}^4\theta^2\right]\Bigg|_{\theta=0}$$
$$= \bar{m}\Sigma\left[1 - \frac{1}{F^2}\left(\frac{1}{2}\sum_{i,j}^{N_f}\left(\frac{\bar{m}}{m_i}+\frac{\bar{m}}{m_j}\right)\Delta(0, M_{ij}^2) - \sum_i^{N_f}\frac{\bar{m}}{m_i}G(0, M_{ii}^2, M_{ii}^2) - 16L_6\sum_i^{N_f}M_{ii}^2 - 16N_f(N_fL_7+L_8)\bar{M}^2\right)\right], \tag{59}$$

where all the masses in the last line are those at $\theta = 0$, or namely $M_{ij}^2 = M_{ij}^2(\theta = 0)$. In the above calculation, we have used the fact that $\sum_i b_i = 0$ [See Eq. (28)]. Note again that the UV divergence is precisely canceled by the renormalization of L_i's and therefore, one can replace $\Delta(0, M^2)$ and L_i's with the renormalized values given in Eqs. (45) and (43), respectively. Since the topological susceptibility is a coefficient of the θ^2 term in the QCD vacuum energy, it does not depend on L_4 and L_5 at NLO, which only appear as corrections to the kinetic term.

B. NLO correction from fixing topology

As discussed above, the next-leading order correction from fixing topology can be calculated at the tree level. The above formula is then simplified:

$$G_Q = G(\theta=0) + \frac{\partial^2}{\partial\theta^2}G(\theta)|_{\theta=0}\frac{1}{2\chi_t V}\left(1 - \frac{Q^2}{\chi_t V}\right) + \text{NNLO terms}, \tag{60}$$

where $\chi_t = \chi_t^{\text{LO}} = \bar{m}\Sigma$ is used. Furthermore, we can ignore all NLO $\times\,\mathcal{O}(\theta^2)$ terms in the correlators $G(\theta)$. Note here that we could have omitted Q^2 term for small Q but kept it, since it gives a $\langle Q^2\rangle = \chi_t V \sim \mathcal{O}(1/p^2)$ contribution when the topology is summed over again in the θ vacuum.

Substituting the expressions in the previous section into Eq. (60), we obtain the correlators in a fixed topological sector of Q:

$$\langle\mathcal{P}\mathcal{P}(t, m_v, m_{v'})\rangle_Q = C_{PP}^Q(m_v, m_{v'})\frac{\cosh(M_{vv'}^Q(t-T/2))}{M_{vv'}^Q\sinh(M_{vv'}^Q T/2)}, \tag{61}$$

$$\langle\mathcal{A}_0\mathcal{P}(t, m_v, m_{v'})\rangle_Q = C_{AP}^Q(m_v, m_{v'}) \times\frac{\sinh(M_{vv'}^Q(t-T/2))}{\sinh(M_{vv'}^Q T/2)}, \tag{62}$$

$$\langle\mathcal{A}_0\mathcal{A}_0(t, m_v, m_{v'})\rangle_Q = C_{AA}^Q(m_v, m_{v'}) \times\frac{M_{vv'}^Q\cosh(M_{vv'}^Q(t-T/2))}{\sinh(M_{vv'}^Q T/2)}, \tag{63}$$

where the valence pion mass at fixed topology is given by

$$(M_{vv'}^Q)^2 = (M_{vv'}^{\text{1-loop}}(\theta=0))^2 \times\left[1 - \frac{1}{2\chi_t V}\left(\frac{\bar{m}^2}{m_v m_{v'}}\right)\left(1 - \frac{Q^2}{\chi_t V}\right)\right], \tag{64}$$

and

$$C_{PP}^Q(m_v, m_{v'}) \equiv \left(\frac{\Sigma_{vv'}^{\text{1-loop}}(\theta=0)}{FZ_F^{vv'}(\theta=0)}\right)^2 \times\left[1 - \frac{1}{4\chi_t V}\left(\frac{\bar{m}}{m_v}+\frac{\bar{m}}{m_{v'}}\right)^2\left(1 - \frac{Q^2}{\chi_t V}\right)\right], \tag{65}$$

$$C_{AP}^Q(m_v, m_{v'}) = \Sigma_{vv'}^{\text{1-loop}}(\theta=0) \times\left[1 - \frac{1}{4\chi_t V}\left(\frac{\bar{m}^2}{m_v^2}+\frac{\bar{m}^2}{m_{v'}^2}\right)\left(1 - \frac{Q^2}{\chi_t V}\right)\right], \tag{66}$$

$$C_{AA}^Q(m_v, m_{v'}) = -(FZ_F^{vv'}(\theta=0))^2 \times\left[1 - \frac{1}{4\chi_t V}\left(\frac{\bar{m}}{m_v}-\frac{\bar{m}}{m_{v'}}\right)^2\left(1 - \frac{Q^2}{\chi_t V}\right)\right], \tag{67}$$

where $\chi_t = \bar{m}\Sigma$. Note that each correction vanishes when summed over the topology, since $\langle Q^2\rangle = \chi_t V$.

From the above Q dependent correlators, the conventional extraction of the pion decay constant, of course, receives a correction from fixing the topology:

$$F^{Q}_{vv'} \equiv \frac{C^{Q}_{AP}(m_v, m_{v'})}{\sqrt{M^{Q}_{vv'} C^{Q}_{PP}(m_v, m_{v'})}} = F Z^{vv'}_{F}(\theta = 0)\left[1 - \frac{1}{8\chi_t V}\left(\frac{\bar{m}}{m_v} - \frac{\bar{m}}{m_{v'}}\right)^2\left(1 - \frac{Q^2}{\chi_t V}\right)\right]. \quad (68)$$

Note that the correction at NLO disappears when $m_v = m_{v'}$.

C. NNLO corrections from fixing topology

In this subsection, we discuss NNLO corrections from fixing topology to the two-point correlators. Here, we do not calculate two-loop diagrams at $\theta = 0$. They are already known in $N_f = 2$ and $2 + 1$ theories [24–31]. Hereafter, we denote them with a superscript "two-loop."

Ignoring the multipion states, the functional form of the correlators at two-loop in the θ vacuum has the following form:

$$G(\theta, t) = C(\theta) f(M(\theta), t), \quad (69)$$

where $C(\theta)$ denotes the time-independent coefficient, while $f(M(\theta), t)$ represents the 1-particle propagator with a mass $M(\theta)$.

In a fixed topological sector, however, the correction can not be factorized as $C^Q \times f(M_Q, t)$ at two-loop level or more. Using notations

$$\delta_Q \equiv \frac{1}{2\chi_t^{\text{1-loop}} V}\left[1 - \frac{Q^2}{\chi_t^{\text{1-loop}} V} - \frac{c_4}{2(\chi_t^{\text{LO}})^2 V}\right],$$
$$O^{(n)}(\theta) \equiv \frac{\partial^n}{\partial \theta^n} O(\theta), \quad (70)$$

for an arbitrary function O of θ, and directly substituting the above expression into Eq. (58), one obtains at NNLO that

$$G_Q(t) = C^Q\left[1 + D^Q \frac{\partial}{\partial M} + \frac{3}{2}(M^{(2)}(0))^2 \delta_Q^2 \frac{\partial^2}{\partial M^2}\right] \times f(M, t)|_{M=M(\theta=0)}, \quad (71)$$

where

$$C^Q \equiv C(0) + C^{(2)}(0)\delta_Q + C^{(4)} \frac{\delta_Q^2}{2}, \quad (72)$$

$$D^Q \equiv M^{(2)}(0)\delta_Q + \left(M^{(4)}(0) + 4M^{(2)}(0)\frac{C^{(2)}(0)}{C(0)}\right)\frac{\delta_Q^2}{2}. \quad (73)$$

Note that due to $C^{(2)}(0)/C(0)$ dependence in D^Q, which is not channel independent, and the second derivative term, the correction in Eq. (71) cannot be simply absorbed into the mass shift in $f(M, t)$.

For more explicit expressions, we have to calculate the 2nd and 4th derivatives of various quantities with respect to θ. We summarize them in Appendix D. Using the notations there, the correlators at NNLO in a fixed topological sector Q are given by

$$\langle \mathcal{J}\mathcal{J}'(t, m_v, m_{v'})\rangle_Q^{\text{NNLO}} = [C^{Q}_{JJ'}(m_v, m_{v'})]^{\text{NNLO}} \times \left[1 + [D^{Q}_{vv'}]_{JJ'} \frac{\partial}{\partial M} + \frac{3}{2}([M^{(2)}_{vv'}]_{\text{LO}})^2 \delta_Q^2 \frac{\partial^2}{\partial M^2}\right] \times f^{JJ'}(M, t)|_{M=M^{\text{2-loop}}_{vv'}(\theta=0)}, \quad (74)$$

$$[D^{Q}_{vv'}]_{JJ'} = [M^{(2)}_{vv'}]_{\text{NLO}}\delta_Q + ([M^{(4)}_{vv'}]_{\text{LO}} + 4[M^{(2)}_{vv'}]_{\text{LO}}[Z^{vv'}_{JJ'}]^{(2)}_{\text{LO}})\frac{\delta_Q^2}{2}, \quad (75)$$

where J and J' represent the operators P or A,

$$f^{PP}(M, t) = \frac{\cosh(M(t - T/2))}{M \sinh(MT/2)}, \quad (76)$$

$$f^{AP}(M, t) = \frac{\sinh(M(t - T/2))}{\sinh(MT/2)}, \quad (77)$$

$$f^{AA}(M, t) = \frac{M\cosh(M(t - T/2))}{\sinh(MT/2)}, \quad (78)$$

and

$$[C^{Q}_{PP}(m_v, m_{v'})]^{\text{NNLO}} = [C^{\theta=0}_{PP}(m_v, m_{v'})]^{\text{2-loop}} \times\left[1 + \left([Z^{vv'}_{PP}]^{(2)}_{\text{NLO}} + \frac{4[Z^{vv'}_{M}]^{(2)}}{Z^{vv'}_{M}(\theta = 0)} + \frac{2[Z^{vv'}_{F}]^{(2)}}{Z^{vv'}_{F}(\theta = 0)}\right)\delta_Q + [Z^{vv'}_{PP}]^{(4)}_{\text{LO}}\frac{\delta_Q^2}{2}\right], \quad (79)$$

$$[C^{Q}_{AP}(m_v, m_{v'})]^{\text{NNLO}} = [C^{\theta=0}_{AP}(m_v, m_{v'})]^{\text{2-loop}} \times\left[1 + \left([Z^{vv'}_{AP}]^{(2)}_{\text{NLO}} + \frac{2[Z^{vv'}_{M}]^{(2)}}{Z^{vv'}_{M}(\theta = 0)} + \frac{2[Z^{vv'}_{F}]^{(2)}}{Z^{vv'}_{F}(\theta = 0)}\right)\delta_Q + [Z^{vv'}_{AP}]^{(4)}_{\text{LO}}\frac{\delta_Q^2}{2}\right], \quad (80)$$

$$[C^{Q}_{AA}(m_v, m_{v'})]^{\rm NNLO} = [C^{\theta=0}_{AA}(m_v, m_{v'})]^{2\text{-loop}} \times\left[1+\left([Z^{vv'}_{AA}]^{(2)}_{\rm NLO}+\frac{2[Z^{vv'}_{F}]^{(2)}}{Z^{vv'}_{F}(\theta=0)}\right)\times\delta_Q+[Z^{vv'}_{AA}]^{(4)}_{\rm LO}\frac{\delta_Q^2}{2}\right]. \tag{81}$$

As is the mass correction, the decay constant at fixed topology is not uniquely extracted from the correlators. If one has a good control of t dependence in Eq. (74) on the lattice, however, a choice is to extract it from the coefficients $[C^Q_{PP}(m_v, m_{v'})]^{\rm NNLO}$ and $[C^Q_{AP}(m_v, m_{v'})]^{\rm NNLO}$ as

$$\frac{[C^{Q}_{AP}(m_v, m_{v'})]^{\rm NNLO}}{\sqrt{[C^{Q}_{PP}(m_v, m_{v'})]^{\rm NNLO}}} = F[Z^{vv'}_{F}(\theta=0)]^{2\text{-loop}}\left[1+\frac{1}{2\chi_t^{1\text{-loop}}V}\left(1-\frac{Q^2}{\chi_t V}-\frac{c_4}{2\chi_t^2 V}\right)\times\left\{[Z^{vv'}_{AP}]^{(2)}_{\rm NLO}-\frac{1}{2}[Z^{vv'}_{PP}]^{(2)}_{\rm NLO}+\frac{[Z^{vv'}_{F}]^{(2)}}{Z^{vv'}_{F}(\theta=0)}\right\}+\frac{1}{8\chi_t^2V^2}\left([Z^{vv'}_{AP}]^{(4)}_{\rm LO}-\frac{1}{2}[Z^{vv'}_{PP}]^{(4)}_{\rm LO}\right)\right]. \tag{82}$$

In spite of a complicated channel dependence and nontrivial t dependence, one can see that the (axial) Ward-Takahashi identity is kept even at fixed topology;

$$\partial_t\langle\mathcal{A}_0\mathcal{P}(t, m_v, m_{v'})\rangle_Q = (m_v + m_{v'})\langle\mathcal{P}\mathcal{P}(t, m_v, m_{v'})\rangle_Q, \tag{83}$$

which can be easily checked by starting from time derivative of the correlator in the θ vacuum, $\partial_t\langle\mathcal{A}_0\mathcal{P}(t, m_v, m_{v'})\rangle_\theta$, and performing integrals over θ.

VI. CONCLUSION

We have discussed ChPT with a nonzero θ term. As a result of CP violation, the vacuum of chiral fields is shifted to a nontrivial element on the $SU(N_f)$ group manifold. We have calculated this vacuum shift at $\mathcal{O}(\theta^3)$ level, as well as the one-loop corrections, from which the topological susceptibility and c_4, the coefficient of θ^4 in the QCD vacuum energy, are extracted.

The CP violation also causes mixing among different CP eigenstates, between scalar and pseudoscalar, or vector and axialvector operators. We have calculated the mesonic two-point functions upto $\mathcal{O}(\theta^2)$ to the one-loop order and θ dependence of the pion mass and decay constant are obtained.

We also have evaluated the effects of fixing topology, by Fourier transform with respect to θ. We found that the effect of fixing topology is considerably suppressed as expected; the tree level diagram only affects on the NLO corrections, one-loop diagram only contributes to the NNLO corrections, and so on.

As applications of this study, it would be interesting to investigate three or four point functions, CP odd observables as well. It would be also important to compare our results with lattice QCD simulations.

ACKNOWLEDGMENTS

The authors thank the member of JLQCD and TWQCD Collaborations for discussions and their encouragement to this study. In particular, S. A. thanks S. Hashimoto and T. Onogi for discussions. H. F. thanks P. H. Damgaard for discussions and many useful comments. The work of S. A. is supported in part by Grants-in-Aid of the Ministry of Education, Culture, Sports, Science and Technology of Japan (Grants No. 20340047, No. 20105001, and No. 20105003). The work of H. F. is supported by the Grant-in-Aid for Nagoya University Global COE Program, "Quest for Fundamental Principles in the Universe: from Particles to the Solar System and the Cosmos," from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

APPENDIX A: EXPLICIT EXPRESSION FOR $G(x, M^2_{ii}, M^2_{jj})$

The diagonal part of the correlator

$$G(x-y, M^2_{ii}(\theta), M^2_{jj}(\theta)) \tag{A1}$$

can be, in principle, expressed in terms of $\Delta(x, M^2)$. In this appendix, we consider the most general case with arbitrary number of flavors. The UV divergence of G at $x = 0$ is also discussed. Furthermore, explicit examples for the degenerate theory and nondegenerate $N_f = N_l + N_s$ flavor case will be given. The similar discussion can be found in Ref. [32]. In the following, for simplicity, we omit the argument θ in $M^2_{ij}(\theta)$. Therefore, M^2_{ij} means $M^2_{ij}(\theta)$, unless explicitly stated.

Let us first define a function

$$f(t) \equiv \frac{1}{N_f}\sum_i^k \frac{n_i}{t - M^2_{ii}}, \tag{A2}$$

where k denotes the number of "different" quark masses, and $n_i \geq 1$ is the degeneracy of the ith mass, which satisfies $\sum_i^k n_i = N_f$. Here, we have ordered the masses $M^2_{ii} < M^2_{i+1i+1}$ for all i. Noting that $f(t)$ is a monotonically decreasing function,

$$\frac{d}{dt}f(t) = -\frac{1}{N_f}\sum_i^k \frac{n_i}{(t-M_{ii}^2)^2} < 0, \quad (A3)$$

and

$$\lim_{\epsilon\to 0} f(M_{ii}^2+\epsilon) = \infty, \qquad \lim_{\epsilon\to 0} f(M_{ii}^2-\epsilon) = -\infty, \quad (A4)$$

$$f(t) < 0, \quad \text{for } t < M_{11}^2 \qquad f(t) > 0, \quad \text{for } M_{kk}^2 < t, \quad (A5)$$

one can show that an equation $f(t) = 0$ has $k-1$ different solutions (we denote them by $t = \hat{M}_{ii}^2$), each of them satisfying

$$M_{ii}^2 < \hat{M}_{ii}^2 < M_{i+1i+1}^2, \qquad (1 \le i \le k-1). \quad (A6)$$

Therefore, $f(-p^2)$ can be written in a rational form:

$$-f(-p^2) = \frac{\prod_i^{k-1}(p^2+\hat{M}_{ii}^2)}{\prod_j^k(p^2+M_{jj}^2)}, \quad (A7)$$

and $G(x, M_{ii}^2, M_{jj}^2)$ can thus be expressed as

$$G(x, M_{ii}^2, M_{jj}^2) = \frac{1}{N_f V}\sum_p \frac{e^{ipx}\prod_f^k(p^2+M_{ff}^2)}{(p^2+M_{ii}^2)(p^2+M_{jj}^2)\prod_f^{k-1}(p^2+\hat{M}_{ff}^2)}$$
$$= \begin{cases} \frac{1}{N_f}[\sum_f^{k-1} A_f^{(ij)}\Delta(x,\hat{M}_{ff}^2) + B_i^{(ij)}\Delta(x,M_{ii}^2) + B_j^{(ij)}\Delta(x,M_{jj}^2)] & (M_{ii}^2 \neq M_{jj}^2), \\ \frac{1}{N_f}[\sum_f^{k-1} A_f^{(ii)}\Delta(x,\hat{M}_{ff}^2) + B^{(ii)}\Delta(x,M_{ii}^2) + C^{(ii)}\partial_{M_{ii}^2}\Delta(x,M_{ii}^2)] & (M_{ii}^2 = M_{jj}^2), \end{cases} \quad (A8)$$

where the coefficients $A_f^{(ij)}$'s, etc. are given by the residues of

$$f_2(t) = \frac{\prod_f^k(-t+M_{ff}^2)}{(-t+M_{ii}^2)(-t+M_{jj}^2)\prod_f^{k-1}(-t+\hat{M}_{ff}^2)}, \quad (A9)$$

[or $-(-t+M_{ii}^2)f_2(t)$ for $C^{(ii)}$], at each pole. Note that $C^{(ii)} = 0$ when M_{ii}^2 is equal to any of the physical masses.

Next, we consider the UV divergence of $G(x = 0, M_{ii}^2, M_{jj}^2)$. By expanding the denominator of Eq. (20) in terms of masses, the UV-divergent part of $G(0, M_{ii}^2, M_{jj}^2)$ can be written as

$$G(0, M_{ii}^2, M_{jj}^2) = \frac{1}{N_f V}\sum_p\left(\frac{1}{p^2} - \frac{M_{ii}^2+M_{jj}^2}{p^4} + \frac{1}{N_f}\sum_f^{N_f}\frac{M_{ff}^2}{p^4} + \cdots\right)$$
$$= -\left(\frac{2}{N_f}M_{ij}^2 - \frac{1}{N_f^2}\sum_f^{N_f}M_{ff}^2\right)\left(\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi\right)/16\pi^2 + \cdots, \quad (A10)$$

where the logarithmic divergence of the last line is canceled by a renormalization of L_i's as seen in Sec. III. Note that the quadratic divergence from $1/p^2$ term is absent in the dimensional regularization.

Here, we give some explicit examples. For the fully degenerate case, i.e., equal masses $M_{ff}^2 = M_{\rm sea}^2$ for all sea flavor f, the above expression for G is greatly simplified,

$$G(x, M_{ii}^2, M_{jj}^2) = \begin{cases} \frac{1}{N_f}[\frac{M_{ii}^2-M_{\rm sea}^2}{M_{ii}^2-M_{jj}^2}\Delta(x,M_{ii}^2) - \frac{M_{jj}^2-M_{\rm sea}^2}{M_{ii}^2-M_{jj}^2}\Delta(x,M_{jj}^2)] & (M_{ii}^2 \neq M_{jj}^2), \\ \frac{1}{N_f}[\Delta(x,M_{ii}^2) - (M_{\rm sea}^2 - M_{ii}^2)\partial_{M_{ii}^2}\Delta(x,M_{ii}^2)] & (M_{ii}^2 = M_{jj}^2). \end{cases} \quad (A11)$$

For the $N_f = N_l + N_s$ flavor theory, where we have N_l quarks of mass m_l and N_s quarks of mass m_s, the equation $f(t) = 0$ is easily solved and one obtains

$$G(x, M_{ii}^2, M_{jj}^2) = \begin{cases} \frac{1}{N_f}[A^{(ij)}\Delta(x,M_\eta^2) + B_i^{(ij)}\Delta(x,M_{ii}^2) + B_j^{(ij)}\Delta(x,M_{jj}^2)] & (M_{ii}^2 \neq M_{jj}^2), \\ \frac{1}{N_f}[A^{(ii)}\Delta(x,M_\eta^2) + B^{(ii)}\Delta(x,M_{ii}^2) + C^{(ii)}\partial_{M^2}\Delta(x,M_{ii}^2)] & (M_{ii}^2 = M_{jj}^2), \end{cases} \quad (A12)$$

where

$$A^{(ij)} = \frac{(M_{ll}^2 - M_\eta^2)(M_{ss}^2 - M_\eta^2)}{(M_{ii}^2 - M_\eta^2)(M_{jj}^2 - M_\eta^2)},$$
$$B_i^{(ij)} = \frac{(M_{ll}^2 - M_{ii}^2)(M_{ss}^2 - M_{ii}^2)}{(M_\eta^2 - M_{ii}^2)(M_{jj}^2 - M_{ii}^2)},$$
$$B_j^{(ij)} = -\frac{(M_{ll}^2 - M_{jj}^2)(M_{ss}^2 - M_{jj}^2)}{(M_\eta^2 - M_{jj}^2)(M_{jj}^2 - M_{ii}^2)}, \tag{A13}$$
$$B^{(ii)} = 1 + \frac{N_l N_s (M_{ll}^2 - M_{ss}^2)^2}{N_f^2 (M_{ii}^2 - M_\eta^2)^2},$$
$$C^{(ii)} = \frac{(M_{ii}^2 - M_{ll}^2)(M_{ii}^2 - M_{ss}^2)}{M_{ii}^2 - M_\eta^2},$$

where $M_{ll}^2 = 2m_l\Sigma/F^2$, $M_{ss}^2 = 2m_s\Sigma/F^2$ and $M_\eta^2 = (N_s M_{ll}^2 + N_l M_{ss}^2)/N_f$.

APPENDIX B: CORRELATORS OF ξ'S AT FINITE VOLUME

In this appendix, we list several useful formulas for the correlation functions of ξ fields or $\Delta(x, M^2)$ at finite volume $V = L^3 T$. In particular, we consider the zero-mode projection or the three-dimensional spatial integrals.

A useful identity is

$$\sum_n \frac{g(\frac{2\pi n}{L}) e^{i((2\pi n)/L)x}}{(\frac{2\pi n}{L})^2 + M^2} = \frac{L}{4M} \frac{1}{\sinh(\frac{ML}{2})} [g(iM) e^{-M(x-L/2)} + g(-iM) e^{M(x-L/2)}], \tag{B1}$$

which holds for an arbitrary regular function $g(p)$. For example, by setting $g = 1$, it is easy to obtain

$$\int d^3x \Delta(x, M^2) = \frac{1}{2M} \frac{\cosh(M(t - T/2))}{\sinh(MT/2)}, \tag{B2}$$

$$\int d^3x \partial_0 \Delta(x, M^2) = \frac{1}{2} \frac{\sinh(M(t - T/2))}{\sinh(MT/2)}, \tag{B3}$$

where we denote $t = x^0$.

Rather nontrivial ones are

$$C_{\Delta^2}(t, M_1^2, M_2^3) \equiv \int d^3x \Delta(x, M_1^2) \Delta(x, M_2^2) = \frac{T}{V} \sum_{\vec{q}=(q_1,q_2,q_3)} \frac{\cosh(|q_1'|(t - T/2))}{2|q_1'| \sinh(|q_1'|T/2)} \times \frac{\cosh(|q_2'|(t - T/2))}{2|q_2'| \sinh(|q_2'|T/2)}, \tag{B4}$$

$$C_{\partial\Delta\Delta}(t, M_1^2, M_2^3) \equiv \int d^3x \partial_0 \Delta(x, M_1^2) \Delta(x, M_2^2) = \frac{T}{V} \sum_{\vec{q}=(q_1,q_2,q_3)} \frac{\sinh(|q_1'|(t - T/2))}{2\sinh(|q_1'|T/2)} \times \frac{\cosh(|q_2'|(t - T/2))}{2|q_2'| \sinh(|q_2'|T/2)}, \tag{B5}$$

$$C_{\partial\Delta\partial\Delta}(t, M_1^2, M_2^3) \equiv \int d^3x \partial_0 \Delta(x, M_1^2) \partial_0 \Delta(x, M_2^2) = \frac{T}{V} \sum_{\vec{q}=(q_1,q_2,q_3)} \frac{\sinh(|q_1'|(t - T/2))}{2\sinh(|q_1'|T/2)} \times \frac{\sinh(|q_2'|(t - T/2))}{2\sinh(|q_2'|T/2)}, \tag{B6}$$

$$C_{\Delta\partial^2\Delta}(t, M_1^2, M_2^3) \equiv \int d^3x \Delta(x, M_1^2) \partial_0^2 \Delta(x, M_2^2) = \frac{T}{V} \sum_{\vec{q}=(q_1,q_2,q_3)} \frac{\cosh(|q_1'|(t - T/2))}{2|q_1'| \sinh(|q_1'|T/2)} \times \frac{|q_2'| \cosh(|q_2'|(t - T/2))}{2\sinh(|q_2'|T/2)}, \tag{B7}$$

where $|q_i'| \equiv \sqrt{\vec{q}^2 + M_i^2}$. As one expects, they are $\mathcal{O}(e^{-(M_1+M_2)t})$ for large T, which describes the two pion state's propagation.

In this paper, we also need

$$C_{\Delta\Delta^2}(t, M_1^2; M_2^2, M_3^2) \equiv \int d^3x \int d^4y \Delta(x - y, M_1^2) \Delta(y, M_2^2) \Delta(y, M_3^2) = \frac{1}{T} \sum_{p_0} \frac{e^{ip_0 t}}{p_0^2 + M_1^2} \times \left[\frac{1}{16\pi^2} \left(\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi \right) + \int_0^1 dx \left(-\frac{\ln F(p_0^2, x, M_2^2, M_3^2) + 1}{16\pi^2} + h^V(x, p_0, F(p_0^2, x, M_2^2, M_3^2)) \right) \right], \tag{B8}$$

and

$$C_{\partial\Delta\Delta\Delta}(t, M_1^2, M_2^2; M_3^2) \equiv \int d^3x \int d^4y \partial_0 \Delta(x-y, M_1^2)\Delta(x-y, M_2^2)\Delta(y, M_3^2)$$
$$= \frac{1}{T}\sum_{p_0} \frac{ip_0 e^{ip_0 t}}{p_0^2 + M_3^2} \times \left[\frac{1}{32\pi^2}\left(\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi\right) + \int_0^1 dx(1-x)\left(-\frac{\ln F(p_0^2, x, M_1^2, M_2^2) + 1}{16\pi^2} + h^V(x, p_0, F(p_0^2, x, M_1^2, M_2^2))\right)\right]. \quad \text{(B9)}$$

Here, $F(p_0^2, x, M_2^2, M_3^2) = x(1-x)p_0^2 + xM_2^2 + (1-x)M_3^2$, and

$$h^V(x, p_0, F) \equiv \sum_{a\neq 0} \int \frac{d^4p'}{(2\pi)^4} \frac{e^{-ip'a}}{\{(p_0' + p_0(x-1/2))^2 + \vec{p}'^2 + F\}^2}$$
$$= -\sum_{a\neq 0} \cos(p_0(x-1/2)a_0) \frac{\partial}{\partial M^2}\left(\frac{M}{4\pi^2|a|}K_1(M|a|)\right)\Bigg|_{M=\sqrt{F}}, \quad \text{(B10)}$$

where the summation is taken over $a_\mu = n_\mu L_\mu$. Note that $h^V(x, p_0, F)$ is exponentially small $\sim \mathcal{O}(e^{-\sqrt{F}L})$. Since both of $\ln F(p_0^2, x, M_2^2, M_3^2)$ and $h^V(x, p_0, F)$ are regular with respect to p_0 for nonzero masses and are symmetric under the flip of $p_0 \to -p_0$, one obtains

$$C_{\Delta\Delta^2}(t, M_1^2; M_2^2, M_3^2) = \frac{1}{2M_1}\frac{\cosh(M_1(t-T/2))}{\sinh(M_1T/2)}\left[\frac{(\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi)}{16\pi^2} + h(M_1^2, M_2^2, M_3^2)\right], \quad \text{(B11)}$$

and

$$C_{\partial\Delta\Delta\Delta}(t, M_1^2, M_2^2; M_3^2) = \frac{\sinh(M_3(t-T/2))}{2\sinh(M_3T/2)}\left[\frac{(\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi)}{32\pi^2} + h'(M_3^2, M_1^2, M_2^2)\right], \quad \text{(B12)}$$

where

$$h(M_1^2, M_2^2, M_3^2) \equiv \int_0^1 dx\left[-\frac{\ln F(-M_1^2, x, M_2^2, M_3^2) + 1}{16\pi^2} - \sum_{a\neq 0}\cosh\left(M_1\left(x - \frac{1}{2}\right)a_0\right)\frac{\partial}{\partial M^2}\left(\frac{M}{4\pi^2|a|}K_1(M|a|)\right)\Bigg|_{M=\sqrt{F(-M_1^2, x, M_2^2, M_3^2)}}\right], \quad \text{(B13)}$$

$$h'(M_3^2, M_1^2, M_2^2) \equiv \int_0^1 dx(1-x)\left[-\frac{\ln F(-M_3^2, x, M_1^2, M_2^2) + 1}{16\pi^2} - \sum_{a\neq 0}\cosh\left(M_3\left(x - \frac{1}{2}\right)a_0\right)\frac{\partial}{\partial M^2}\left(\frac{M}{4\pi^2|a|}K_1(M|a|)\right)\Bigg|_{M=\sqrt{F(-M_3^2, x, M_1^2, M_2^2)}}\right]. \quad \text{(B14)}$$

Note that the logarithmic divergences are canceled by the renormalization of L_i's (See Appendix C).

APPENDIX C: DETAILS OF TWO-POINT CORRELATORS

In this appendix, we list several equations which are needed to calculate Eqs. (53)–(55). We first define

$$X_{ij}(x) \equiv \sum_f^{N_f} \Delta(x, M_{if}^2)\Delta(x, M_{jf}^2) - \Delta(x, M_{ij}^2)G(x, M_{ii}^2, M_{ii}^2) - \Delta(x, M_{ij}^2)G(x, M_{jj}^2, M_{jj}^2) - 2\Delta(x, M_{ij}^2)G(x, M_{ii}^2, M_{jj}^2), \quad \text{(C1)}$$

$$\begin{aligned}Y_0^{ij}(x) \equiv \sum_f^{N_f}[&\partial_0\Delta(x, M_{if}^2)\Delta(x, M_{jf}^2)\\ &- \partial_0\Delta(x, M_{jf}^2)\Delta(x, M_{if}^2)]\\ &- \Delta(x, M_{ij}^2)\partial_0[G(x, M_{ii}^2, M_{ii}^2) - G(x, M_{jj}^2, M_{jj}^2)]\\ &+ \partial_0\Delta(x, M_{ij}^2)[G(x, M_{ii}^2, M_{ii}^2) - G(x, M_{jj}^2, M_{jj}^2)],\end{aligned} \tag{C2}$$

$$\begin{aligned}W_{00}^{ij}(x) \equiv \sum_f^{N_f}[&\partial_0^2\Delta(x, M_{jf}^2)\Delta(x, M_{if}^2)\\ &+ \partial_0^2\Delta(x, M_{if}^2)\Delta(x, M_{jf}^2)\\ &- 2\partial_0\Delta(x, M_{if}^2)\partial_0\Delta(x, M_{jf}^2)]\\ &+ 2\partial_0^2\Delta(x, M_{ij}^2)A(x, M_{ii}^2, M_{jj}^2)\\ &+ 2\Delta(x, M_{ij}^2)\partial_0^2A(x, M_{ii}^2, M_{jj}^2)\\ &- 4\partial_0\Delta(x, M_{ij}^2)\partial_0A(x, M_{ii}^2, M_{jj}^2).\end{aligned} \tag{C3}$$

In the above expressions, we have omitted the argument θ in the mass unless its difference from $M_{ij}^2(\theta = 0)$ is important. Note that Y_0^{ij} is always finite and $Y_0^{ij} = 0$ when $m_i = m_j$.

Using the formulas in Appendix B, we can perform the zero momentum projection in a finite volume. It is straightforward to obtain

$$C_X^{ij}(t) \equiv \int d^3x X_{ij}(x), \qquad C_{Y_0}^{ij}(t) \equiv \int d^3x Y_0^{ij}(x), \qquad C_{W_{00}}^{ij}(t) \equiv \int d^3x W_{00}^{ij}(x). \tag{C4}$$

For example, $C_X^{ij}(t)$ is explicitly given by

$$\begin{aligned}C_X^{ij}(t) &\equiv \int d^3x X_{ij}(x)\\ &= \sum_f^{N_f} C_{\Delta^2}(t, M_{if}^2, M_{jf}^2) - \frac{1}{N_f}\left(\sum_l^{k-1} A_l^{(ii)} C_{\Delta^2}(t, M_{ij}^2, \hat{M}_{ll}^2) + B^{(ii)} C_{\Delta^2}(t, M_{ij}^2, M_{ii}^2) + C^{(ii)}\partial_{M^2} C_{\Delta^2}(t, M_{ij}^2, M^2)|_{M=M_{ii}}\right)\\ &\quad - \frac{1}{N_f}\left(\sum_l^{k-1} A_l^{(jj)} C_{\Delta^2}(t, M_{ij}^2, \hat{M}_{ll}^2) + B^{(jj)} C_{\Delta^2}(t, M_{ij}^2, M_{jj}^2) + C^{(jj)}\partial_{M^2} C_{\Delta^2}(t, M_{ij}^2, M^2)|_{M=M_{jj}}\right)\\ &\quad - \frac{2}{N_f}\left(\sum_l^{k-1} A_l^{(ij)} C_{\Delta^2}(t, M_{ij}^2, \hat{M}_{ll}^2) + B_i^{(ij)} C_{\Delta^2}(t, M_{ij}^2, M_{ii}^2) + B_j^{(ij)} C_{\Delta^2}(t, M_{ij}^2, M_{jj}^2)\right),\end{aligned} \tag{C5}$$

where k is the number of different sea quark masses, and the coefficients A, B, C's and $\hat{M}_{ll}^2$ are given in Appendix A.

Rather nontrivial integrals are

$$\int d^3x \int d^4y \Delta(x - y, M_{ij}^2) X_{ij}(y) = \frac{1}{2M_{ij}} \frac{\cosh(M_{ij}(t - T/2))}{\sinh(M_{ij}T/2)} \left[\left(\frac{N_f}{2} - \frac{2}{N_f}\right) \frac{\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi}{8\pi^2} + H_{ij}(M_{ij}^2)\right], \tag{C6}$$

$$\begin{aligned}&\int d^3x \int d^4y d^4z \Delta(x - y, M_{ij}^2) X_{ij}(y - z) \Delta(z, M_{ij}^2)\\ &= \left(-\frac{1}{2M}\frac{\partial}{\partial M}\right)\left\{\frac{1}{2M}\frac{\cosh(M(t - T/2))}{\sinh(MT/2)}\left[\left(\frac{N_f}{2} - \frac{2}{N_f}\right)\frac{\frac{1}{\epsilon} + 1 - \gamma + \ln 4\pi}{8\pi^2} + H_{ij}(M^2)\right]\right\}\Bigg|_{M=M_{ij}},\end{aligned} \tag{C7}$$

and

$$\int d^3x \int d^4y Y_0^{ij}(x - y)\Delta(y, M_{ij}^2) = \frac{1}{2}\frac{\sinh(M_{ij}(t - T/2))}{\sinh(M_{ij}T/2)} H'_{ij}(M_{ij}^2), \tag{C8}$$

where

$$H_{ij}(M^2) \equiv \sum_f^{N_f} h(M^2, M_{if}^2, M_{jf}^2) - \frac{1}{N_f}\left[\sum_l^{k-1}(A_l^{(ii)} + A_l^{(jj)} + 2A_l^{(ij)})h(M^2, M_{ij}^2, \hat{M}_{ll}^2) + (B^{(ii)} + 2B_i^{(ij)})h(M^2, M_{ij}^2, M_{ii}^2) + (B^{(jj)} + 2B_j^{(ij)})h(M^2, M_{ij}^2, M_{jj}^2) + C^{(ii)}\partial_{M_*^2}h(M^2, M_{ij}^2, M_*^2)|_{M_*=M_{ii}} + C^{(jj)}\partial_{M_*^2}h(M^2, M_{ij}^2, M_*^2)|_{M_*=M_{jj}}\right], \quad \text{(C9)}$$

$$H'_{ij}(M^2) \equiv \sum_f^{N_f}[h'(M^2, M_{if}^2, M_{jf}^2) - h'(M^2, M_{jf}^2, M_{if}^2)] + \frac{1}{N_f}\left[\sum_l^{k-1}(A_l^{(ii)} - A_l^{(jj)})(h'(M^2, M_{ij}^2, \hat{M}_{ll}^2) - h'(M^2, \hat{M}_{ll}^2, M_{ij}^2)) + B^{(ii)}(h'(M^2, M_{ij}^2, M_{ii}^2) - h'(M^2, M_{ii}^2, M_{ij}^2)) - B^{(jj)}(h'(M^2, M_{ij}^2, M_{jj}^2) - h'(M^2, M_{jj}^2, M_{ij}^2)) + C^{(ii)}\partial_{M_*^2}(h'(M^2, M_{ij}^2, M_*^2) - h'(M^2, M_*^2, M_{ij}^2))|_{M_*=M_{ii}} - C^{(jj)}\partial_{M_*^2}(h'(M^2, M_{ij}^2, M_*^2) - h'(M^2, M_*^2, M_{ij}^2))|_{M_*=M_{jj}}\right]. \quad \text{(C10)}$$

Note that $1/\epsilon$ divergence is canceled by the renormalization of L_7 and L_8.

Finally, we present the overall coefficients in Eqs. (53)–(55):

$$[C_{PP}^\theta(m_v, m_{v'})]^{1\text{-loop}} \equiv \frac{(\Sigma_{vv'}^{1\text{-loop}}(\theta))^2}{(FZ_F^{vv'}(\theta))^2} Z_{PP}^{vv'}(\theta), \quad \text{(C11)}$$

$$[C_{AP}^\theta(m_v, m_{v'})]^{1\text{-loop}} \equiv \Sigma_{vv'}^{1\text{-loop}}(\theta) Z_{AP}^{vv'}(\theta), \quad \text{(C12)}$$

$$[C_{AA}^\theta(m_v, m_{v'})]^{1\text{-loop}} \equiv -(FZ_F^{vv'}(\theta))^2 Z_{AA}^{vv'}(\theta), \quad \text{(C13)}$$

where we have defined $\Sigma_{vv'}^{1\text{-loop}}(\theta) \equiv \Sigma(Z_M^{vv'}(\theta)Z_F^{vv'}(\theta))^2$ and dimensionless coefficients Z's are given by

$$Z_{PP}^{vv'}(\theta) \equiv \frac{1 + \cos(\theta_v + \theta_{v'})}{2} - \frac{\bar{M}^4\theta^2}{2F^2}\left(\frac{\partial}{\partial M^2}H_{vv'}^r(M^2, \mu_{\text{sub}})|_{M=M_{vv'}}\right) - \frac{\bar{M}^2\theta}{2F^2}(\theta_v + \theta_{v'})\{32(N_f L_7^r(\mu_{\text{sub}}) + L_8^r(\mu_{\text{sub}})) + H_{vv'}^r(M_{vv'}^2, \mu_{\text{sub}}))\}, \quad \text{(C14)}$$

$$Z_{AP}^{vv'}(\theta) \equiv \frac{\cos\theta_v + \cos\theta_{v'}}{2} - \frac{\bar{M}^4\theta^2}{2F^2}\left(\frac{\partial}{\partial M^2}H_{vv'}^r(M^2, \mu_{\text{sub}})|_{M=M_{vv'}}\right) - \frac{\bar{M}^2\theta}{4F^2}(\theta_v + \theta_{v'})\{32(N_f L_7^r(\mu_{\text{sub}}) + L_8^r(\mu_{\text{sub}})) + H_{vv'}^r(M_{vv'}^2, \mu_{\text{sub}}))\} + \frac{1}{4}(\theta_v - \theta_{v'})\frac{\bar{M}^2\theta}{F^2}H'_{vv'}(M_{vv'}^2), \quad \text{(C15)}$$

$$Z_{AA}^{vv'}(\theta) \equiv \frac{1 + \cos(\theta_v - \theta_{v'})}{2} - \frac{\bar{M}^4\theta^2}{2F^2}\left(\frac{\partial}{\partial M^2}H_{vv'}^r(M^2, \mu_{\text{sub}})|_{M=M_{vv'}}\right) + \frac{1}{2}(\theta_v - \theta_{v'})\frac{\bar{M}^2\theta}{F^2}H'_{vv'}(M_{vv'}^2), \quad \text{(C16)}$$

where $L_7^r(\mu_{\text{sub}})$, $L_8^r(\mu_{\text{sub}})$ and

$$H_{vv'}^r(M_{vv'}^2, \mu_{\text{sub}}) \equiv H_{vv'}(M_{vv'}^2) + \frac{1}{8\pi^2}\left(\frac{N_f}{2} - \frac{2}{N_f}\right)\ln\mu_{\text{sub}}^2 \quad \text{(C17)}$$

represent the renormalized values at a reference scale μ_{sub}. In these functions one can ignore the argument θ of the masses and just put $M_{vv'}^2 = M_{vv'}^2(\theta = 0)$, since they only appear in $\mathcal{O}(\theta^2) \times \mathcal{O}(p^2)$ terms.

APPENDIX D: θ DERIVATIVES

In this appendix, we list the θ derivatives of various quantities, which are needed to evaluate those in a fixed topological sector shown in Sec. V. Here, we evaluate them at NLO for the second derivatives while at LO for the 4th derivatives.

For the mass matrix, we obtain

$$[M_{ij}^{(2)}]_{\text{LO}} \equiv \frac{\partial^2}{\partial\theta^2}M_{ij}(\theta)|_{\theta=0} = -M_{ij}\left(\frac{\bar{m}^2}{2m_i m_j}\right), \quad \text{(D1)}$$

$$[M_{ij}^{(4)}]_{\text{LO}} \equiv \frac{\partial^4}{\partial\theta^4}M_{ij}(\theta)|_{\theta=0} = \frac{\bar{M}^2}{4M_{ij}}\left[\frac{\bar{m}^3}{m_i^3} + \frac{\bar{m}^3}{m_j^3} + 24(a_i + a_j)\right] - \frac{3M_{ij}}{4}\left(\frac{\bar{m}^2}{m_i m_J}\right)^2, \quad \text{(D2)}$$

where the argument $\theta = 0$ is omitted.

For the one-loop propagator, or the chiral-log terms, we have

$$\Delta^{(2)}(0, M_{ij}^2) \equiv -M_{ij}^2\left(\frac{\bar{m}^2}{m_i m_j}\right)\partial_{M^2}\Delta(0, M^2)|_{M=M_{ij}}. \quad \text{(D3)}$$

Using this, it is straightforward to calculate

$$G^{(2)}(0, M_{ii}^2, M_{jj}^2) \equiv \frac{\partial^2}{\partial\theta^2}G(0, M_{ii}^2(\theta), M_{jj}^2(\theta)), \quad \text{(D4)}$$

$$A^{(2)}(0, M_{ii}^2, M_{jj}^2) \equiv G^{(2)}(0, M_{ii}^2, M_{jj}^2) - \tfrac{1}{2}(G^{(2)}(0, M_{ii}^2, M_{ii}^2) + G^{(2)}(0, M_{jj}^2, M_{jj}^2)), \quad \text{(D5)}$$

and

$$[Z_M^{ij}]^{(2)} \equiv \frac{1}{2F^2}\bigg[G^{(2)}(0, M_{ii}^2, M_{jj}^2) + 8(L_4 - 2L_6) \times \sum_f^{N_f} M_{ff}^2\left(\frac{\bar{m}^2}{m_f^2}\right) + 8(L_5 - 2L_8)M_{ij}^2\left(\frac{\bar{m}^2}{m_i m_j}\right)\bigg], \quad \text{(D6)}$$

$$[Z_F^{ij}]^{(2)} \equiv -\frac{1}{2F^2}\bigg[\frac{\sum_f^{N_f}(\Delta^{(2)}(0, M_{if}^2) + \Delta^{(2)}(0, M_{jf}^2))}{2} + A^{(2)}(0, M_{ii}^2, M_{jj}^2) + 8\left(L_4\sum_f^{N_f} M_{ff}^2\frac{\bar{m}^2}{m_f^2} + L_5 M_{ij}^2\left(\frac{\bar{m}^2}{m_i m_j}\right)\right)\bigg]. \quad \text{(D7)}$$

It is then easy to obtain the second derivative of the mass at NLO:

$$[M_{ij}^{(2)}]_{\rm NLO} = M_{ij}^{\text{1-loop}}(\theta = 0)\bigg[-\left(\frac{\bar{m}^2}{2m_i m_j}\right) + \frac{\bar{M}^2}{2M_{ij}^2}(b_i + b_j) + \frac{[Z_M^{ij}]^{(2)}}{Z_M^{ij}(\theta = 0)} - \frac{\bar{M}^4\{32(N_f L_7^r(\mu_{\rm sub}) + L_8^r(\mu_{\rm sub})) + H_{ij}^r(M_{ij}^2, \mu_{\rm sub})\}}{2F^2 M_{ij}^2}\bigg]. \quad \text{(D8)}$$

For the overall coefficients of the correlators, we have

$$[Z_{PP}^{vv'}]_{\rm LO}^{(2)} \equiv -\frac{1}{2}\left(\frac{\bar{m}}{m_v} + \frac{\bar{m}}{m_{v'}}\right)^2, \quad \text{(D9)}$$

$$[Z_{PP}^{vv'}]_{\rm NLO}^{(2)} \equiv [Z_{PP}^{vv'}]_{\rm LO}^{(2)} + \left(\frac{\bar{m}}{m_v} + \frac{\bar{m}}{m_{v'}}\right)(b_v + b_{v'}) - \frac{\bar{M}^2}{F^2}\bigg[\bar{M}^2\partial_{M^2}H_{vv'}^r(M^2, \mu_{\rm sub}) + \left(\frac{\bar{m}}{m_v} + \frac{\bar{m}}{m_{v'}}\right)\{32(N_f L_7^r(\mu_{\rm sub}) + L_8^r(\mu_{\rm sub})) + H_{vv'}^r(M_{vv'}^2, \mu_{\rm sub})\}\bigg], \quad \text{(D10)}$$

$$[Z_{AP}^{vv'}]_{\rm LO}^{(2)} \equiv -\frac{1}{2}\left(\frac{\bar{m}^2}{m_v^2} + \frac{\bar{m}^2}{m_{v'}^2}\right), \quad \text{(D11)}$$

$$[Z_{AP}^{vv'}]_{\rm NLO}^{(2)} \equiv [Z_{AP}^{vv'}]_{\rm LO}^{(2)} + \left(\frac{\bar{m}}{m_v}b_v + \frac{\bar{m}}{m_{v'}}b_{v'}\right) - \frac{\bar{M}^2}{F^2}\bigg[\bar{M}^2\partial_{M^2}H_{vv'}^r(M^2, \mu_{\rm sub}) + \frac{1}{2}\left(\frac{\bar{m}}{m_v} + \frac{\bar{m}}{m_{v'}}\right)\{32(N_f L_7^r(\mu_{\rm sub}) + L_8^r(\mu_{\rm sub})) + H_{vv'}^r(M_{vv'}^2, \mu_{\rm sub})\} - \frac{1}{2}\left(\frac{\bar{m}}{m_v} - \frac{\bar{m}}{m_{v'}}\right)H'_{vv'}(M_{vv'}^2)\bigg], \quad \text{(D12)}$$

$$[Z_{AA}^{vv'}]_{\rm LO}^{(2)} \equiv -\frac{1}{2}\left(\frac{\bar{m}}{m_v} - \frac{\bar{m}}{m_{v'}}\right)^2, \quad \text{(D13)}$$

$$[Z_{AA}^{vv'}]_{\rm NLO}^{(2)} \equiv [Z_{AA}^{vv'}]_{\rm LO}^{(2)} + \left(\frac{\bar{m}}{m_v} - \frac{\bar{m}}{m_{v'}}\right)(b_v - b_{v'}) - \frac{\bar{M}^2}{F^2}\bigg[\bar{M}^2\partial_{M^2}H_{vv'}^r(M^2, \mu_{\rm sub}) - \left(\frac{\bar{m}}{m_v} - \frac{\bar{m}}{m_{v'}}\right)H'_{vv'}(M_{vv'}^2)\bigg]. \quad \text{(D14)}$$

Their 4th derivatives are given by

$$[Z_{PP}^{vv'}]^{(4)}_{\rm LO} \equiv \frac{1}{2}\left(\frac{\bar{m}}{m_v}+\frac{\bar{m}}{m_{v'}}\right)\left[\left(\frac{\bar{m}}{m_v}+\frac{\bar{m}}{m_{v'}}\right)^3 + 24(a_v + a_{v'})\right], \tag{D15}$$

$$[Z_{AP}^{vv'}]^{(4)}_{\rm LO} \equiv \frac{1}{2}\left[\left(\frac{\bar{m}^4}{m_v^4}+\frac{\bar{m}^4}{m_{v'}^4}\right) + 24\left(\frac{\bar{m}}{m_v}a_v + \frac{\bar{m}}{m_{v'}}a_{v'}\right)\right], \tag{D16}$$

$$[Z_{AA}^{vv'}]^{(4)}_{\rm LO} \equiv \frac{1}{2}\left(\frac{\bar{m}}{m_v}-\frac{\bar{m}}{m_{v'}}\right)\left[\left(\frac{\bar{m}}{m_v}-\frac{\bar{m}}{m_{v'}}\right)^3 + 24(a_v - a_{v'})\right]. \tag{D17}$$

[1] Latest results from large scale full QCD simulations can be found in Ph. Boucaud *et al.* (ETM Collaboration), Phys. Lett. B **650**, 304 (2007); S. Aoki *et al.* (JLQCD Collaboration), Phys. Rev. D **78**, 014508 (2008); C. Allton *et al.* (RBC-UKQCD Collaboration), Phys. Rev. D **78**, 114509 (2008); S. Aoki *et al.* (PACS-CS Collaboration), Phys. Rev. D **79**, 034503 (2009).

[2] S. Weinberg, Phys. Rev. **166**, 1568 (1968).

[3] J. Gasser and H. Leutwyler, Ann. Phys. (N.Y.) **158**, 142 (1984); Nucl. Phys. **B250**, 465 (1985).

[4] For the recent review on the θ vacuum, see E. Vicari and H. Panagopoulos, Phys. Rep. **470**, 93 (2009).

[5] R. F. Dashen, Phys. Rev. D **3**, 1879 (1971).

[6] E. Witten, Ann. Phys. (N.Y.) **128**, 363 (1980); P. Di Vecchia and G. Veneziano, Nucl. Phys. **B171**, 253 (1980); M. Creutz, Phys. Rev. D **52**, 2951 (1995); A. V. Smilga, Phys. Rev. D **59**, 114021 (1999).

[7] V. Baluni, Phys. Rev. D **19**, 2227 (1979); R. J. Crewther, P. Di Vecchia, G. Veneziano, and E. Witten, Phys. Lett. **88B**, 123 (1979); **91B**, 487(E) (1980); M. Pospelov and A. Ritz, Phys. Rev. Lett. **83**, 2526 (1999); B. Borasoy, Phys. Rev. D **61**, 114017 (2000); P. Faccioli, D. Guadagnoli, and S. Simula, Phys. Rev. D **70**, 074017 (2004).

[8] S. Aoki and A. Gocksch, Phys. Rev. Lett. **63**, 1125 (1989); **65**, 1172(E) (1990); S. Aoki, A. Gocksch, A. V. Manohar, and S. R. Sharpe, Phys. Rev. Lett. **65**, 1092 (1990).

[9] E. Shintani *et al.*, Phys. Rev. D **72**, 014504 (2005); F. Berruto, T. Blum, K. Orginos, and A. Soni, Phys. Rev. D **73**, 054509 (2006); L. Del Debbio, G. M. Manca, H. Panagopoulos, A. Skouroupathis, and E. Vicari, J. High Energy Phys. 06 (2006) 005; E. Shintani *et al.*, Phys. Rev. D **75**, 034507 (2007); L. Giusti, S. Petrarca, and B. Taglienti, Phys. Rev. D **76**, 094510 (2007); E. Shintani, S. Aoki, and Y. Kuramashi, Phys. Rev. D **78**, 014503 (2008).

[10] H. Fukaya and T. Onogi, Phys. Rev. D **70**, 054508 (2004).

[11] R. Brower, S. Chandrasekharan, J. W. Negele, and U. J. Wiese, Phys. Lett. B **560**, 64 (2003).

[12] S. Aoki, H. Fukaya, S. Hashimoto, and T. Onogi, Phys. Rev. D **76**, 054508 (2007).

[13] H. Neuberger, Phys. Lett. B **417**, 141 (1998); **427**, 353 (1998).

[14] T. Izubuchi and C. Dawson (RBC Collaboration), Nucl. Phys. B, Proc. Suppl. **106**, 748 (2002); P. M. Vranas, Phys. Rev. D **74**, 034512 (2006); H. Fukaya *et al.* (JLQCD Collaboration), Phys. Rev. D **74**, 094505 (2006); D. Renfrew, T. Blum, N. Christ, R. Mawhinney, and P. Vranas, Proc. Sci. LATTICE2008 (2008) 048; F. Bruckmann, F. Gruber, K. Jansen, M. Marinkovic, C. Urbach, and M. Wagner, arXiv:0905.2849.

[15] H. Fukaya *et al.* (JLQCD Collaboration), Phys. Rev. Lett. **98**, 172001 (2007); Phys. Rev. D **76**, 054503 (2007).

[16] H. Fukaya *et al.* (JLQCD collaboration), Phys. Rev. D **77**, 074503 (2008); J. Noaki *et al.* (JLQCD and TWQCD Collaborations), Phys. Rev. Lett. **101**, 202004 (2008).

[17] S. Aoki *et al.* (JLQCD and TWQCD Collaborations), Phys. Lett. B **665**, 294 (2008).

[18] F. C. Hansen, Nucl. Phys. **B345**, 685 (1990); F. C. Hansen and H. Leutwyler, Nucl. Phys. **B350**, 201 (1991); H. Leutwyler and A. V. Smilga, Phys. Rev. D **46**, 5607 (1992); K. Splittorff and J. J. M. Verbaarschot, Phys. Rev. Lett. **90**, 041601 (2003); Y. V. Fyodorov and G. Akemann, JETP Lett. **77**, 438 (2003); K. Splittorff and J. J. M. Verbaarschot, Nucl. Phys. **B683**, 467 (2004).

[19] S. R. Sharpe, Phys. Rev. D **56**, 7052 (1997); **62**, 099901(E) (2000); M. F. L. Golterman and K. C. L. Leung, Phys. Rev. D **57**, 5703 (1998); P. H. Damgaard and K. Splittorff, Phys. Rev. D **62**, 054509 (2000); S. R. Sharpe and N. Shoresh, Phys. Rev. D **64**, 114510 (2001); J. Bijnens and T. A. Lahde, Phys. Rev. D **71**, 094502 (2005); J. Bijnens, N. Danielsson, and T. A. Lahde, Phys. Rev. D **73**, 074509 (2006).

[20] J. Lenaghan and T. Wilke, Nucl. Phys. **B624**, 253 (2002).

[21] Y. Y. Mao and T. W. Chiu (TWQCD Collaboration), Phys. Rev. D **80**, 034502 (2009).

[22] J. Wess and B. Zumino, Phys. Lett. **37B**, 95 (1971); E. Witten, Nucl. Phys. **B223**, 422 (1983).

[23] C. Bernard (MILC Collaboration), Phys. Rev. D **65**, 054031 (2002).

[24] J. Bijnens, N. Danielsson, and T. A. Lahde, Phys. Rev. D **70**, 111503 (2004).

[25] J. Bijnens, N. Danielsson, and T. A. Lahde, Phys. Rev. D **73**, 074509 (2006).

[26] J. Bijnens, G. Colangelo, and G. Ecker, Ann. Phys. (N.Y.) **280**, 100 (2000).

[27] G. Colangelo and C. Haefeli, Nucl. Phys. **B744**, 14 (2006).

[28] G. Amoros, J. Bijnens, and P. Talavera, Nucl. Phys. **B568**, 319 (2000).
[29] E. Golowich and J. Kambor, Phys. Rev. D **58**, 036004 (1998).
[30] G. Amoros, J. Bijnens, and P. Talavera, Nucl. Phys. **B602**, 87 (2001).
[31] R. Kaiser, J. High Energy Phys. 09 (2007) 065.
[32] P. H. Damgaard and H. Fukaya, J. High Energy Phys. 01 (2009) 052.