Finite volume QCD at fixed topological charge

Sinya Aoki,[1,2] Hidenori Fukaya,[3] Shoji Hashimoto,[4,5] and Tetsuya Onogi[6]

[1]*Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Ibaraki Japan*
[2]*Riken BNL Research Center, Brookhaven National Laboratory, Upton, New York 11973, USA*
[3]*Theoretical Physics Laboratory, RIKEN, Wako 351-0198, Japan*
[4]*High Energy Accelerator Research Organization (KEK), Tsukuba 305-0801, Japan*
[5]*School of High Energy Accelerator Science, The Graduate University for Advanced Studies (Sokendai), Tsukuba 305-0801, Japan*
[6]*Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*

In finite volume the partition function of QCD with a given θ is a sum of different topological sectors with a weight primarily determined by the topological susceptibility. If a physical observable is evaluated only in a fixed topological sector, the result deviates from the true expectation value by an amount proportional to the inverse space-time volume $1/V$. Using the saddle point expansion, we derive formulas to express the correction due to the fixed topological charge in terms of a $1/V$ expansion. Applying this formula, we propose a class of methods to determine the topological susceptibility in QCD from various correlation functions calculated in a fixed topological sector.

I. INTRODUCTION

Quantum chromodynamics (QCD) in four space-time dimensions allows topologically nontrivial gauge configurations labeled by a winding number or a topological charge Q. The path integral to define the partition function of QCD includes an integral over configurations with arbitrary Q. In order to ensure the cluster decomposition property of physical observables, the weight among different topological sectors must be $e^{i\theta Q}$, which defines the θ vacuum of QCD. If one considers a path integral restricted in a fixed topological sector, the cluster decomposition property—one of the necessary properties of quantum field theory—is violated [1]. In this paper we address the question of fixing topology in the context of nonperturbative calculation of QCD on the lattice. But the analysis does not depend on any particular regularization of the theory.

In the lattice QCD simulations the inclusion of the effects of dynamical quarks is computationally most demanding. Since the direct computation of the fermion determinant $\det(D + m)^2$, with D the Dirac operator on the lattice and m the quark mass, requires prohibitive computational cost, one usually introduces a pseudofermion field ϕ to write the determinant in the form $\int[d\phi] \times [d\phi^\dagger] \exp(-\phi^\dagger(D + m)^{-2}\phi)$, so that the problem is reduced to an evaluation of the inverse fermion matrix $(D + m)^{-1}$. Since the effective lattice action becomes nonlocal, the Monte Carlo updation is most efficiently done by updating all the gauge links on the lattice at the same time introducing a molecular dynamics evolution. The most popular such algorithm to date is the hybrid Monte Carlo algorithm [2] that combines the molecular dynamics evolution with a Metropolis accept/reject step.

With the molecular dynamics evolution, the ergodicity becomes a potential problem when there exist more than one region of phase space that are separated by some potential wall, because the "kinetic energy" of the molecular dynamics system may not be enough to go through the potential wall. This situation happens for QCD in four dimensions because of the nontrivial topological sectors. In the continuum theory the potential barrier is infinite and the gauge configurations in different topological sectors cannot be reached by a single stream of the continuous evolution. On the lattice, the potential barrier is finite (order of inverse lattice spacing $1/a$) and the probability of tunneling among different topological sectors is nonzero, but will exponentially drop ($\sim e^{-U_0/a}$ with U_0/a a nominal potential height) as the continuum limit is approached. This means that the correct sampling of topological charge and thus the valid simulation of the θ vacuum of QCD will become increasingly more difficult [3,4]. In fact, this problem already manifests itself in the recent dynamical overlap fermion simulations by the JLQCD Collaboration [5–8], since they explicitly introduce a term that prevents topology change [9] in order to avoid large numerical cost due to the discontinuity of the overlap operator along the topology boundary.

One may then ask whether lattice QCD simulations with a fixed topological charge are useful, in general, to extract physics of real world, i.e. QCD at a given value of θ. (If the CP symmetry is preserved, $\theta = 0$. Small but nonzero θ implies an interesting physics case to give rise to the neutron electric dipole moment.) The fixed topology simulation is desirable in the study of the ϵ regime of QCD, since the physical quantities have striking dependence on the topological charge, which is an important part of the physics we are interested in. (For a recent unquenched lattice simulation in the ϵ regime, see [10,11].) But in the p regime, the fixed topology simulation gives rise to a systematic effect. In this paper we try to answer this question theoretically without relying on any particular model

or assumption. Extending a previous work by Brower *et al.* [12], we show that observables calculated at a fixed topological charge are different from those at $\theta = 0$ by an amount of order of inverse space-time volume $1/V$, so that both agree in the infinite volume limit.

This result can be understood intuitively within the instanton picture of the topological excitation in the QCD vacuum. The instanton is a local object carrying a unit topological charge. Starting from a trivial topological sector, an instanton and anti-instanton can be pair-created or annihilated without changing the net topology and then may be separated from each other. If we look at a region (or subvolume) including the (anti-)instanton, that region has locally nontrivial topological charge. In this way, the topological fluctuation may occur even if the net topological charge is kept fixed. Supporting evidence of this expectation has been found in the chirality density of low-lying eigenmodes of the overlap-Dirac operator; i.e. local chirality is strongly peaked at ± 1 even on the gauge configurations with net topological charge $Q = 0$ [6]. The effect of fixing the net topology will become relatively small as the total volume becomes larger, as there is more chance to create (or annihilate) the instanton–anti-instanton pairs. The topological susceptibility χ_t characterizes the magnitude of these local topological fluctuations.

In fact, in our formulation the topological susceptibility enters in the difference of $O(1/V)$ between the fixed topological sector and the fixed θ vacuum. This type of finite volume effect can even be evaluated, once we know the coefficient of $1/V$, which is found, in general, to be a second derivative of the physical quantity of interest with respect to θ, as well as the topological susceptibility χ_t. In this paper, we describe the method to extract χ_t from a gauge ensemble in the fixed topological sector, leaving the estimate of the finite size effects for other physical quantities for a future publication.

This paper is organized as follows. In Sec. II, by using the saddle point expansion, we derive a formula which expresses the partition function at a fixed topological charge in terms of the partition function at $\theta = 0$ and its derivatives with respect to θ. We extend this formula to the case for arbitrary correlation functions. From these results it is easy to show that arbitrary correlation functions at fixed topological charge agree with those at $\theta = 0$ in the infinite volume limit. In Sec. III, as an application of the above formulas, we show that the topological susceptibility χ_t can be extracted from the two-point function of the topological charge density at a fixed topological charge. Through the Ward-Takahashi (WT) identities, we then relate the two-point function of the topological charge density with a two-point function of the pseudoscalar density, which is more suitable for actual calculations with the overlap fermions. An extension to the case of four- and three-point correlation functions is also discussed. In Sec. IV, we consider a case of *CP*-odd observ-

ables, taking the calculation of the neutron electric dipole moment as an example. Our conclusion is given in Sec. V. In Appendix A we check the validity of the saddle point expansion, by comparing the expansion with an exact calculation for a simple example. Results at order V^{-3} are summarized in Appendix B.

II. GENERAL FORMULA

A. Partition function at a fixed topological charge

We first consider the partition function in the θ vacuum defined by

$$Z(\theta) \equiv \langle \theta | \theta \rangle = \exp[-VE(\theta)], \qquad (1)$$

where $E(\theta)$ is the energy per (space-time) volume V. Without loss of generality we take $Z(0) = 1$ as a normalization, which is equivalent to $E(0) = 0$. $E(\theta)$ satisfies the conditions $E(\theta + 2\pi) = E(\theta) = E(-\theta)$. The topological susceptibility χ_t at $\theta = 0$ is defined by

$$\chi_t = \frac{\langle 0 | Q^2 | 0 \rangle}{V}, \qquad (2)$$

which is obtained by a second derivative of $E(\theta)$,

$$\chi_t = \frac{d^2 E(\theta)}{d\theta^2} \bigg|_{\theta=0}. \qquad (3)$$

Since $\chi_t \geq 0$ by definition, $\theta = 0$ is a local minimum of $E(\theta)$. Moreover, Vafa and Witten proved that $Z(0) > Z(\theta)$ [13], which leads to $E(0) < E(\theta)$ for $\forall \theta \neq 0$. Namely, $\theta = 0$ is the global minimum of the function $E(\theta)$. While we assume that $E(\theta)$ is analytic at $\theta = 0$, $E(\theta)$ may have a nonanalyticity at $\theta \neq 0$, in particular, at $\theta = \pi$. For instance, chiral perturbation theory (ChPT) at the leading order gives

$$E(\theta) = \chi_t N_f^2 [1 - \cos(\theta/N_f)], \qquad -\pi < \theta \leq \pi \quad (4)$$

for N_f number of flavors. A θ derivative of this particular form is discontinuous at $\theta = \pm \pi$ for $N_f > 1$ [14]. From these general conditions we can expand $E(\theta)$ around $\theta = 0$,

$$E(\theta) = \sum_{n=1}^{\infty} \frac{c_{2n}}{(2n)!} \theta^{2n} = \frac{\chi_t}{2} \theta^2 + O(\theta^4). \qquad (5)$$

The partition function at a fixed topological charge Q is a Fourier coefficient of the periodic function $Z(\theta)$,

$$\begin{aligned} Z_Q &= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta Z(\theta) \exp(i\theta Q) \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \exp(-VF(\theta)), \end{aligned} \qquad (6)$$

where $F(\theta) \equiv E(\theta) - i\theta Q/V$, and the Fourier expansion of $Z(\theta)$ is written as

$$Z(\theta) = \sum_{Q=0,\pm1,\pm2,\cdots} Z_Q e^{-i\theta Q}. \tag{7}$$

For a large enough volume, we can evaluate the θ integral in (6) by the saddle point expansion. The saddle point θ_c is given by

$$\theta_c = i\frac{Q}{\chi_t V}(1 + O(\delta^2)) \tag{8}$$

where $\delta \equiv Q/(\chi_t V)$. We then expand $F(\theta)$ as

$$F(\theta) = F(\theta_c) + \frac{E^{(2)}}{2}(\theta_c)(\theta - \theta_c)^2$$
$$+ \sum_{n=3}^{\infty} \frac{E^{(n)}(\theta_c)}{n!}(\theta - \theta_c)^n, \tag{9}$$

where $E^{(n)}$ is the nth derivative of $E(\theta)$ with respect to θ at $\theta = \theta_c$, and is given by

$$VF(\theta_c) = \frac{Q^2}{2\chi_t V}(1 + O(\delta^2)), \tag{10}$$

$$E^{(2)}(\theta_c) = \chi_t(1 + O(\delta^2)), \tag{11}$$

$$E^{(2n)}(\theta_c) = c_{2n}(1 + O(\delta^2)), \tag{12}$$

$$E^{(2n-1)}(\theta_c) = \theta_c c_{2n}(1 + O(\delta^2)). \tag{13}$$

Hereafter we omit an argument θ_c of $E^{(n)}(\theta_c)$ and simply write it as $E^{(n)}$ unless otherwise stated. By a change of variable $s = \sqrt{E^{(2)}V}(\theta - \theta_c)$ we can rewrite the integral as

$$\begin{aligned}
Z_Q &= \frac{e^{-VF(\theta_c)}}{2\pi\sqrt{E^{(2)}V}} \int_{\sqrt{E^{(2)}V}(-\pi-\theta_c)}^{\sqrt{E^{(2)}V}(\pi-\theta_c)} ds \exp\left[-\frac{s^2}{2} - \sum_{n=3} \frac{E^{(n)}V}{n!}\left(\frac{s}{\sqrt{E^{(2)}V}}\right)^n\right] \\
&= \frac{e^{-VF(\theta_c)}}{2\pi\sqrt{E^{(2)}V}} \int_{-\infty}^{\infty} ds \exp\left[-\frac{s^2}{2} - \sum_{n=3} \frac{E^{(n)}V}{n!}\left(\frac{s}{\sqrt{E^{(2)}V}}\right)^n\right] + O(e^{-V}) \\
&= \frac{e^{-VF(\theta_c)}}{\sqrt{2\pi E^{(2)}V}} \left\langle \exp\left[-\sum_{n=3} \frac{E^{(n)}V}{n!}\left(\frac{s}{\sqrt{E^{(2)}V}}\right)^n\right]\right\rangle + O(e^{-V}). \tag{14}
\end{aligned}$$

We defined

$$\langle f(s)\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\, e^{-s^2/2} f(s), \tag{15}$$

with which $\langle s^{2n}\rangle = (2n-1)!!$. Neglecting exponentially suppressed terms and expanding in powers of $1/V$, we obtain

$$\begin{aligned}
Z_Q &= \frac{e^{-VF(\theta_c)}}{\sqrt{2\pi E^{(2)}V}}\left[1 - \left\langle\sum_{n=3} \frac{E^{(n)}V}{n!}\left(\frac{s}{\sqrt{E^{(2)}V}}\right)^n\right\rangle + \cdots\right] \\
&= \frac{e^{-VF(\theta_c)}}{\sqrt{2\pi E^{(2)}V}}\left[1 - \frac{E^{(4)}V}{8(E^{(2)}V)^2} + O\left(\frac{1}{V^2}\right)\right] \\
&= \frac{1}{\sqrt{2\pi\chi_t V}}\exp\left[-\frac{Q^2}{2\chi_t V}\right]\left[1 - \frac{c_4}{8V\chi_t^2} + O\left(\frac{1}{V^2}, \delta^2\right)\right]. \tag{16}
\end{aligned}$$

This shows that, as long as $\delta \ll 1$ (equivalently, $Q \ll \chi_t V$), the distribution of Q becomes the Gaussian distribution. Note, however, that the distribution can deviate from a Gaussian for $Q = O(V)$, as numerically observed on a quenched lattice [15–18].

B. Correlation functions

Here we consider an arbitrary correlation function

$$G(\theta) = \langle\theta|O_1 O_2 \cdots O_n|\theta\rangle, \tag{17}$$

whose Fourier coefficient at a fixed topological charge Q is

defined by

$$G_Q = \frac{1}{Z_Q}\frac{1}{2\pi}\int d\theta Z(\theta)G(\theta)\exp(i\theta Q). \tag{18}$$

Note that the operators O_i do not contain θ, and the θ dependence comes solely from the vacuum angle. Using the saddle point expansion as before, we obtain

$$\begin{aligned}
G_Q &= \frac{1}{Z_Q}\frac{e^{-VF(\theta_c)}}{2\pi\sqrt{E^{(2)}V}}\int_{-\infty}^{\infty} ds \exp\left[-\frac{s^2}{2} - \sum_{n=3}^{\infty}\frac{E^{(n)}V}{n!}\right. \\
&\quad \left.\times\left(\frac{s}{\sqrt{E^{(2)}V}}\right)^n\right]G\left(\theta_c + \frac{s}{\sqrt{E^{(2)}V}}\right) \\
&= G(\theta_c) + \sum_{k=1}^{\infty} G^{(k)}(\theta_c)\frac{1}{k!}\left\langle\!\left\langle\left(\frac{s}{\sqrt{E^{(2)}V}}\right)^k\right\rangle\!\right\rangle, \tag{19}
\end{aligned}$$

where we define

$$\begin{aligned}
\langle\!\langle f(s)\rangle\!\rangle &\equiv \frac{1}{Z_Q}\frac{e^{-VF(\theta_c)}}{2\pi\sqrt{E^{(2)}V}}\int_{-\infty}^{\infty} ds\, f(s) \\
&\quad \times \exp\left[-\frac{s^2}{2} - \sum_{n=3}^{\infty}\frac{E^{(n)}V}{n!}\left(\frac{s}{\sqrt{E^{(2)}V}}\right)^n\right] \tag{20}
\end{aligned}$$

and $G^{(n)}$ is the nth derivative of G with respect to θ. Using the formulas

$$\langle\!\langle 1\rangle\!\rangle = 1, \tag{21}$$

$$\langle\langle s^2 \rangle\rangle = 1 - \frac{E^{(4)}V}{2(E^{(2)}V)^2} + \frac{5(E^{(3)}V)^2}{4(E^{(2)}V)^3} + O(V^{-2}), \tag{22}$$

$$\langle\langle s^4 \rangle\rangle = 3!! + O(V^{-1}), \tag{23}$$

$$\langle\langle s \rangle\rangle = -\frac{E^{(3)}V}{2(E^{(2)}V)^{3/2}}\left(1 - \frac{4E^{(4)}V}{3(E^{(2)}V)^2} + \frac{5(E^{(3)}V)^2}{4(E^{(2)}V)^3}\right) - \frac{E^{(5)}V}{8(E^{(2)}V)^{5/2}} + O(V^{-5/2}), \tag{24}$$

$$\langle\langle s^3 \rangle\rangle = -\frac{5E^{(3)}V}{2(E^{(2)}V)^{3/2}} + O(V^{-3/2}), \tag{25}$$

we finally obtain

$$G_Q = G(\theta_c) + G^{(2)}(\theta_c)\frac{1}{2E^{(2)}V}\left(1 - \frac{E^{(4)}V}{2(E^{(2)}V)^2} + \frac{5(E^{(3)}V)^2}{4(E^{(2)}V)^3}\right) + G^{(4)}(\theta_c)\frac{1}{8(E^{(2)}V)^2}$$
$$- G^{(1)}(\theta_c)\left[\frac{E^{(3)}V}{2(E^{(2)}V)^2}\left(1 - \frac{4E^{(4)}V}{3(E^{(2)}V)^2} + \frac{5(E^{(3)}V)^2}{4(E^{(2)}V)^3}\right) + \frac{E^{(5)}V}{8(E^{(2)}V)^3}\right] - G^{(3)}(\theta_c)\frac{5E^{(3)}V}{12(E^{(2)}V)^3} + O(V^{-3}). \tag{26}$$

The above expansion is valid for any θ_c as long as $G^{(n)}(\theta_c)/G(\theta_c) = O(1)$ as $V \to \infty$.

Depending on the size of θ_c, we can further expand the above formula. If we take $\theta_c = O(V^{-1})$ [equivalently, $Q = O(1)$], we have

$$G_Q = G(0) + G^{(1)}(0)\theta_c + G^{(2)}(0)\frac{\theta_c^2}{2} + G^{(2)}(0)\frac{1}{2E^{(2)}V}\left(1 - \frac{E^{(4)}V}{2(E^{(2)}V)^2}\right) + G^{(3)}\frac{\theta_c}{2E^{(2)}V} + G^{(4)}(0)\frac{1}{8(E^{(2)}V)^2}$$
$$- G^{(1)}(0)\left[\frac{E^{(3)}V}{2(E^{(2)}V)^2}\left(1 - \frac{4E^{(4)}V}{3(E^{(2)}V)^2}\right) + \frac{E^{(5)}V}{8(E^{(2)}V)^3}\right] - G^{(2)}(0)\theta_c\frac{E^{(3)}V}{2(E^{(2)}V)^2} + O(V^{-3})$$
$$= G(0) + G^{(2)}(0)\frac{1}{2\chi_t V}\left[1 - \frac{Q^2}{\chi_t V} - \frac{c_4}{2\chi_t^2 V}\right] + G^{(4)}(0)\frac{1}{8\chi_t^2 V^2} + G^{(1)}(0)\frac{iQ}{\chi_t V}\left(1 - \frac{c_4}{2\chi_t^2 V}\right) + G^{(3)}(0)\frac{iQ}{2\chi_t^2 V^2} + O(V^{-3}). \tag{27}$$

If G is CP even, G is an even function of θ, so that

$$G_Q^{\text{even}} = G(0) + G^{(2)}(0)\frac{1}{2\chi_t V}\left[1 - \frac{Q^2}{\chi_t V} - \frac{c_4}{2\chi_t^2 V}\right]$$
$$+ G^{(4)}(0)\frac{1}{8\chi_t^2 V^2} + O(V^{-3}), \tag{28}$$

while, if G is CP odd, we have

$$G_Q^{\text{odd}} = G^{(1)}(0)\frac{iQ}{\chi_t V}\left(1 - \frac{c_4}{2\chi_t^2 V}\right) + G^{(3)}(0)\frac{iQ}{2\chi_t^2 V^2}$$
$$+ O(V^{-3}). \tag{29}$$

In order to claim that the above expansion is convergent, $G^{(n)}(0)/G(\theta)$ must be $O(1)$. This condition is satisfied because the expansion

$$G(\theta) = G(0) + \sum_{n=1}^{\infty} G^{(n)}(0)\frac{\theta^n}{n!} \tag{30}$$

is valid for $\forall \theta = O(1)$.

The formula (28) provides an estimate of the finite size effect due to the fixed topological charge. The leading correction is of order $O(1/V)$ as advertised. The dimension is compensated by the topological susceptibility χ_t. In ChPT it is evaluated as $\chi_t = m\Sigma/N_f$ by the sea quark mass m and the chiral condensate Σ as well as the number of flavors N_f [19]. The finite volume correction is suppressed when the quark mass is larger than $1/(\Sigma V)$, while it becomes significant when $m \sim 1/(\Sigma V)$. This is consistent with the fact that the topological charge has a strong effect in the ϵ regime, which is characterized by $m\Sigma V \lesssim 1$. The correction has a coefficient $G^{(2)}(0)$ that represents the θ dependence of the correlator. This is not known, in general, but can be fitted with lattice data at various Q. In the mass region where ChPT is applicable, it can also be estimated, as done in [12] at the tree level for pseudoscalar meson mass. One-loop calculations are in progress.

The other interesting formula (29) suggests a possibility to calculate CP-odd observables, such as the neutron elec-

tric dipole moment, at a fixed nonzero topological charge, which will be discussed in Sec. IV.

III. TOPOLOGICAL SUSCEPTIBILITY

In this section, we propose methods to extract the topological susceptibility χ_t from correlation functions at a fixed topological charge Q.

A. Two-point correlation function

1. Bosonic formula

Suppose that there is a well-defined local operator $\omega(x)$ that measures the local topological charge. The global topological charge Q is then obtained as $Q = \int d^4x \omega(x)$, and the topological susceptibility is $\chi_t = \int d^4x \langle \omega(x)\omega(0) \rangle$, where the expectation value is taken for the $\theta = 0$ vacuum.

Since $\omega(x)\omega(0)$ is CP even, Eq. (28) gives

$$\langle \omega(x)\omega(0)\rangle_Q = \langle \omega(x)\omega(0)\rangle + \langle \omega(x)\omega(0)\rangle^{(2)}\frac{1}{2V\chi_t}$$

$$\times \left(1 - \frac{Q^2}{V\chi_t} - \frac{c_4}{2\chi_t^2 V}\right)$$

$$+ \langle \omega(x)\omega(0)\rangle^{(4)}\frac{1}{8\chi_t^2 V^2} + O(V^{-3}). \quad (31)$$

Here $\langle \mathcal{O} \rangle$ means a vacuum expectation value of $\mathcal{O}$ at $\theta = 0$ and $\langle \mathcal{O} \rangle^{(n)}$ denotes its nth derivative with respect to θ. In the large separation limit $|x| \to \infty$, the CP invariance at $\theta = 0$ and the clustering property at a fixed θ [1] gives

$$\langle \omega(x)\omega(0)\rangle \to \langle \omega(x)\rangle\langle \omega(0)\rangle = 0. \quad (32)$$

In addition,

$$\langle \omega(x)\omega(0)\rangle^{(2)} = -\langle \omega(x)\omega(0)Q^2\rangle + \langle \omega(x)\omega(0)\rangle\langle Q^2\rangle, \quad (33)$$

whose second term vanishes as $|x| \to \infty$. Denoting a connected vacuum expectation value (VEV) as $\langle \cdots \rangle_c$, the first term can be written as

$$\int d^4y d^4z \langle \omega(x)\omega(0)\omega(y)\omega(z)\rangle$$

$$= \int d^4y d^4z [\langle \omega(x)\omega(0)\omega(y)\omega(z)\rangle_c + \langle \omega(x)\omega(0)\rangle$$

$$\times \langle \omega(y)\omega(z)\rangle + \langle \omega(x)\omega(y)\rangle\langle \omega(0)\omega(z)\rangle$$

$$+ \langle \omega(x)\omega(z)\rangle\langle \omega(y)\omega(0)\rangle].$$

As $|x| \to \infty$, the first and the second terms vanish and we obtain

$$\int d^4y \int d^4z \langle \omega(x)\omega(y)\rangle\langle \omega(z)\omega(0)\rangle + (y \leftrightarrow z)$$

$$= 2\int d^4y \langle \omega(y)\omega(0)\rangle \int d^4z \langle \omega(x)\omega(z)\rangle. \quad (34)$$

Using the translational invariance, this becomes $2\chi_t^2$. Therefore, the term $\langle \omega(x)\omega(0)\rangle^{(2)}$ in (31) gives $-2\chi_t^2$ in the large separation limit.

Similarly, we consider

$$\langle \omega(x)\omega(0)\rangle^{(4)} = \langle \omega(x)\omega(0)Q^4\rangle - 6\langle \omega(x)\omega(0)Q^2\rangle\langle Q^2\rangle$$

$$+ \langle \omega(x)\omega(0)\rangle\{6\langle Q^2\rangle^2 - \langle Q^4\rangle\}. \quad (35)$$

The first term is written as

$$\langle \omega(x)\omega(0)Q^4\rangle = \int \prod_i d^4x_i \langle \omega(x)\omega(0)\omega(x_1)\omega(x_2)\omega(x_3)$$

$$\times \omega(x_4)\rangle, \quad (36)$$

which may be decomposed in terms of the connected VEVs. Since the terms containing both $\omega(x)$ and $\omega(0)$ in the same connected VEV vanish, only the following terms remain:

$$\int \prod_i d^4x_i [8\langle \omega(x)\omega(x_1)\omega(x_2)\omega(x_3)\rangle_c\langle \omega(0)\omega(x_4)\rangle$$

$$+ 12\langle \omega(x)\omega(x_1)\rangle\langle \omega(x_2)\omega(x_3)\rangle\langle \omega(0)\omega(x_4)\rangle]$$

$$= 8\chi_t\frac{\langle Q^4\rangle_c}{V} + 12V\chi_t^3. \quad (37)$$

Putting this into (35) we have

$$\langle \omega(x)\omega(0)\rangle^{(4)} \to 8\chi_t\frac{\langle Q^4\rangle_c}{V} = \frac{8\chi_t}{V}\frac{d^4}{d\theta^4}\log Z(\theta) = -8\chi_t c_4 \quad (38)$$

for the fourth-derivative term in (31).

Gathering all terms we arrive at

$$\lim_{|x| \to \text{large}} \langle \omega(x)\omega(0)\rangle_Q = \frac{1}{V}\left(\frac{Q^2}{V} - \chi_t - \frac{c_4}{2\chi_t V}\right) + O(V^{-3})$$

$$+ O(e^{-m_{\eta'}|x|}), \quad (39)$$

where the flavor singlet pseudoscalar meson mass, $m_{\eta'}$, is the lightest mass of possible intermediate states. This result explicitly shows that QCD at a fixed topological charge (in a finite volume) is sick as a quantum field theory, because the clustering property is violated. However, the magnitude of the violation can be estimated as a $1/V$ expansion without introducing strong assumptions on the details of the dynamics of QCD. The same result (up to the c_4 term) was obtained in the context of a two-dimensional model in [20].

Physical quantities such as the topological susceptibility χ_t can be obtained through (39). In practice, this formula will be used for a finite separation x instead of $|x| \to \infty$. The clustering property (32) in the θ vacuum receives a correction of order of $e^{-m_{\eta'}|x|}$, which vanishes quickly because the flavor singlet meson η' acquires a large mass due to the axial anomaly of QCD.

2. Fermionic formula

We now express the bosonic correlation function $\langle\omega(x)\omega(0)\rangle$ in terms of a fermionic one using the anomalous axial U(1) WT identities for an arbitrary operator O:

$$\langle\partial_\mu A_\mu(x)O - 2mP(x)O + 2\omega(x)O + \delta_x O\rangle = 0, \quad (40)$$

where $A_\mu(x) = \frac{1}{N_f}\sum_f\bar{\psi}^f(x)\gamma_\mu\gamma_5\psi^f(x)$ and $P(x) = \frac{1}{N_f}\sum_f\bar{\psi}^f(x)\gamma_5\psi^f(x)$ are the flavor singlet axial-vector current and pseudoscalar density, respectively, and $\delta_x O$ denotes an axial rotation of the operator O at x. Here the quark field has a flavor index f running from 1 to N_f. The expectation value $\langle\cdots\rangle$ in (40) can be taken either in the θ vacuum or in the fixed Q sector, since the WT identities are valid with any external states. Combining the following two WT identities [for $O = 2mP(0)$ and $O = 2\omega(x)$ with $x \neq 0$],

$$\langle 2mP(x)2mP(0)\rangle = \langle\partial_\mu A_\mu(x)2mP(0)\rangle + \langle 2\omega(x)2mP(0)\rangle, \quad (41)$$

$$\langle 2\omega(x)2mP(0)\rangle = \langle 2\omega(x)\partial_\mu A_\mu(0)\rangle + \langle 2\omega(x)2\omega(0)\rangle, \quad (42)$$

we obtain a relation at a fixed topological charge,

$$\begin{aligned}\langle 2mP(x)2mP(0)\rangle_Q &= \langle 2\omega(x)2\omega(0)\rangle_Q \\ &+ \langle\partial_\mu A_\mu(x)2mP(0)\rangle_Q \\ &+ \langle 2\omega(x)\partial_\mu A_\mu(0)\rangle_Q. \quad (43)\end{aligned}$$

In the large separation limit $|x|\to\infty$, using (28) the second term becomes

$$\begin{aligned}\langle\partial_\mu A_\mu(x)2mP(0)\rangle_Q &\to \langle\partial_\mu A_\mu(x)\rangle\langle 2mP(0)\rangle \\ &+ \frac{1}{2V\chi_t}\left(1 - \frac{Q^2}{V\chi_t} - \frac{c_4}{2\chi_t^2 V}\right) \\ &\times \langle\partial_\mu A_\mu(x)2mP(0)\rangle^{(2)} \\ &+ \frac{1}{8\chi_t^2 V^2}\langle\partial_\mu A_\mu(x)2mP(0)\rangle^{(4)}.\end{aligned}$$
$$(44)$$

The first term on the right-hand side vanishes, and the second term is evaluated as

$$\begin{aligned}\langle\partial_\mu A_\mu(x)2mP(0)\rangle^{(2)} &= \langle\partial_\mu A_\mu(x)2mP(0)Q^2\rangle \\ &\to 2\langle\partial_\mu A_\mu(x)Q\rangle\langle 2mP(0)Q\rangle. \quad (45)\end{aligned}$$

Since the translational invariance (plus an appropriate boundary condition) leads to

$$\langle\partial_\mu A_\mu(x)Q\rangle = \frac{1}{V}\int d^4x\langle\partial_\mu A_\mu(x)Q\rangle = 0, \quad (46)$$

we obtain $\langle\partial_\mu A_\mu(x)2mP(0)\rangle^{(2)} = 0$ in the large separation limit.

We next consider the fourth-derivative term. In general,

$$\begin{aligned}\langle A(x)B(0)\rangle^{(4)} &= \langle A(x)B(0)Q^4\rangle - 6\langle A(x)B(0)Q^2\rangle\langle Q^2\rangle \\ &+ \langle A(x)B(0)\rangle\{6\langle Q^2\rangle^2 - \langle Q^4\rangle\} \quad (47)\end{aligned}$$

when $\langle A(x)\rangle = \langle B(0)\rangle = 0$. Using relations

$$\langle A(x)B(0)Q^2\rangle \to 2\langle A(x)Q\rangle_c\langle B(0)Q\rangle_c, \quad (48)$$

$$\begin{aligned}\langle A(x)B(0)Q^4\rangle &= \langle A(x)B(0)Q^4\rangle_c + \langle A(x)B(0)\rangle_c\langle Q^4\rangle_c \\ &+ 6\langle A(x)B(0)Q^2\rangle_c\langle Q^2\rangle_c \\ &+ 3\langle A(x)B(0)\rangle_c\langle Q^2\rangle_c^2 \\ &+ 4\langle A(x)Q\rangle_c\langle B(0)Q^3\rangle_c \\ &+ 4\langle B(0)Q\rangle_c\langle A(x)Q^3\rangle_c \\ &+ 12\langle A(x)Q\rangle_c\langle B(0)Q\rangle_c\langle Q^2\rangle_c \\ &\to 4\langle A(x)Q\rangle_c\langle B(0)Q^3\rangle_c \\ &+ 4\langle B(0)Q\rangle_c\langle A(x)Q^3\rangle_c \\ &+ 12\langle A(x)Q\rangle_c\langle B(0)Q\rangle_c\langle Q^2\rangle_c, \quad (49)\end{aligned}$$

the general formula reads

$$\begin{aligned}\langle A(x)B(0)\rangle^{(4)} &\to 4\langle A(x)Q\rangle_c\langle B(0)Q^3\rangle_c + 4\langle B(0)Q\rangle_c \\ &\times\langle A(x)Q^3\rangle_c. \quad (50)\end{aligned}$$

For $A(x) = \partial_\mu A_\mu(x)$, the translational invariance again gives $\langle A(x)Q\rangle_c = \langle A(x)Q^3\rangle_c = 0$, and therefore $\langle\partial_\mu A_\mu(x)2mP(0)\rangle^{(4)} \to 0$. We thus conclude that the term $\langle\partial_\mu A_\mu(x)2mP(0)\rangle_Q$ on the right-hand side of (43) vanishes in the large separation limit $|x|\to\infty$, and the same conclusion also holds for the last term $\langle 2\omega(x)\partial_\mu A_\mu(0)\rangle_Q$ in (43).

Combining these, we finally obtain

$$\begin{aligned}\lim_{|x|\to\text{large}}\langle mP(x)mP(0)\rangle_Q &= \lim_{|x|\to\text{large}}\langle\omega(x)\omega(0)\rangle_Q \\ &= \frac{1}{V}\left(\frac{Q^2}{V} - \chi_t - \frac{c_4}{2\chi_t V}\right) \\ &+ O(e^{-m_{\eta'}|x|}). \quad (51)\end{aligned}$$

Namely, the topological susceptibility can also be calculated with the singlet pseudoscalar density correlator at a fixed topology. If we apply the above evaluation to the nonsinglet WT identities, we can show

$$\begin{aligned}\lim_{|x|\to\text{large}}\langle 2mP^a(x)2mP^a(0)\rangle_Q &= \lim_{|x|\to\text{large}}\langle\partial_\mu A_\mu^a(x)2mP^a(0)\rangle_Q \\ &= 0, \quad (52)\end{aligned}$$

where $A_\mu^a(x) = \bar{\psi}(x)\gamma_\mu\gamma_5 T^a\psi(x)$ and $P^a = \bar{\psi}(x)\gamma_5 T^a\psi(x)$ are the flavor nonsinglet axial-vector current and pseudoscalar density, respectively, with $\text{tr}\,T^a = 0$ and $\text{tr}\,(T^a T^b) = \delta^{ab}/N_f$. By subtracting this equation from (51), we may write

$$\lim_{|x| \to \text{large}} \langle mP(x)mP(0) \rangle_Q^{\text{disc}} \equiv \lim_{|x| \to \text{large}} [\langle mP(x)mP(0) \rangle_Q$$

$$- \langle mP^a(x)mP^a(0) \rangle_Q]$$

$$= \frac{1}{V} \left(\frac{Q^2}{V} - \chi_t - \frac{c_4}{2\chi_t V} \right)$$

$$+ O(e^{-m_\pi |x|}), \quad (53)$$

where the superscript ''disc'' represents a disconnected contribution, and no summation is taken here for a. Since the large separation limit of the nonsinglet correlator (52) is saturated only after a slowly dumping factor $e^{-m_\pi |x|}$ with the pion mass m_π, the singlet correlator (51) is preferable for practical use.

B. Four-point correlation function

Here we extend our analysis to a four-point function.

1. Bosonic formula

We consider a CP-even observable

$$\langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle_Q = \langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle$$

$$+ \langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle^{(2)}$$

$$\times \frac{1}{2V\chi_t} \left(1 - \frac{Q^2}{V\chi_t} - \frac{c_4}{2\chi_t^2 V} \right)$$

$$+ \langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle^{(4)}$$

$$\times \frac{1}{8\chi_t^2 V^2} + O(V^{-3}). \quad (54)$$

We assume that four topological charge density operators are far apart from any others ($|x_i - x_j| \to$ large for $\forall i \neq \forall j$). In this limit both $\langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle$ and $\langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle^{(2)}$ vanish and $\langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle^{(4)}$ becomes $24\chi_t^4$, taking the procedure used to obtain the analogous formula (38) in the two-point function case. We obtain

$$\langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle_Q$$

$$= 3 \frac{\chi_t^2}{V^2} \left[1 + \frac{1}{\chi_t^2 V} (c_4 - Q^2 \chi_t) \right]^2 + O(V^{-4}). \quad (55)$$

In addition to the leading $O(1/V^2)$ term, we also give a next-to-leading $O(1/V^3)$ correction. Details of this $O(1/V^3)$ calculation are given in Appendix B.

2. Fermionic formula

Again we use the anomalous axial WT identities, which give a chain of equations,

$$\langle P_1 P_2 P_3 P_4 \rangle = \langle dA_1 P_2 P_3 P_4 \rangle + \langle \omega_1 P_2 P_3 P_4 \rangle, \quad (56)$$

$$\langle \omega_1 P_2 P_3 P_4 \rangle = \langle dA_2 \omega_1 P_3 P_4 \rangle + \langle \omega_1 \omega_2 P_3 P_4 \rangle, \quad (57)$$

$$\langle \omega_1 \omega_2 P_3 P_4 \rangle = \langle dA_3 \omega_1 \omega_2 P_4 \rangle + \langle \omega_1 \omega_2 \omega_3 P_4 \rangle, \quad (58)$$

$$\langle \omega_1 \omega_2 \omega_3 P_4 \rangle = \langle dA_4 \omega_1 \omega_2 \omega_3 \rangle + \langle \omega_1 \omega_2 \omega_3 \omega_4 \rangle, \quad (59)$$

where we have used a shorthand notation, $P_i \equiv mP(x_i)$, $dA_i \equiv \partial_\mu A_\mu(x_i)/2$, and $\omega_i \equiv \omega(x_i)$. The operators are far apart from others, as before. Since the WT identities are valid in the fixed topological sector, we obtain

$$\langle P_1 P_2 P_3 P_4 \rangle_Q = \langle \omega_1 \omega_2 \omega_3 \omega_4 \rangle_Q + \langle dA_1 P_2 P_3 P_4$$

$$+ \omega_1 dA_2 P_3 P_4 + \omega_1 \omega_2 dA_3 P_4$$

$$+ \omega_1 \omega_2 \omega_3 dA_4 \rangle_Q. \quad (60)$$

From the clustering property and CP invariance the correlator $\langle dA_i O_{jkl} \rangle$ vanishes, where $O_{jkl} \equiv F_j F_k F_l$ with $F_i = P_i$ or ω_i (i, j, k, l are all different). In addition, $\langle dA_i O_{jkl} \rangle^{(2)}$ vanishes, because it is written as $-\langle dA_i O_{jkl} Q^2 \rangle \to -\langle dA_i Q \rangle \langle O_{jkl} Q \rangle$. Similarly, $\langle dA_i O_{jkl} \rangle^{(4)}$ vanishes, because it is $\langle dA_i O_{jkl} Q^4 \rangle \to 4 \langle dA_i Q \rangle \langle O_{jkl} Q^3 \rangle$ and $\langle \partial_\mu A(x) Q \rangle = (1/V) \int d^4x \langle \partial_\mu A(x) Q \rangle = 0$. We therefore obtain $\langle dA_i O_{jkl} \rangle_Q \to 0$, which leads to

$$\langle P_1 P_2 P_3 P_4 \rangle_Q \to \langle \omega_1 \omega_2 \omega_3 \omega_4 \rangle_Q$$

$$= 3 \frac{\chi_t^2}{V^2} \left[1 + \frac{1}{\chi_t^2 V} (c_4 - Q^2 \chi_t) \right]^2 + O(V^{-4}). \quad (61)$$

Similarly the nonsinglet WT identities imply that $\langle P_i^a P_j^a P_k P_l \rangle_Q$ and $\langle P_i^a P_j^a P_k^b P_l^b \rangle_Q$ vanish in the large separation limit, where $P_i^a = P^a(x_i)$ is a nonsinglet pseudoscalar density and i, j, k, l are all different from others. We then conclude that the disconnected correlator has the same asymptotic form as $\langle \omega_1 \omega_2 \omega_3 \omega_4 \rangle_Q$:

$$\langle P_1 P_2 P_3 P_4 \rangle_Q^{\text{disc}} \equiv \langle P_1 P_2 P_3 P_4 \rangle_Q - \{ \langle P_1^a P_2^a P_3 P_4 \rangle_Q$$

$$+ \langle P_1 P_2 P_3^a P_4^a \rangle_Q - \langle P_1^a P_2^a P_3^b P_4^b \rangle_Q \}$$

$$- \{2 \leftrightarrow 3\} - \{2 \leftrightarrow 4\}$$

$$\to 3 \frac{\chi_t^2}{V^2} \left[1 + \frac{1}{\chi_t^2 V} (c_4 - Q^2 \chi_t) \right]^2$$

$$+ O(V^{-4}), \quad (62)$$

where no sum is taken for $a \neq b$.

The formulas (55) and (62) provide another method to extract the topological susceptibility from a fixed topological sector. Since the contamination from the higher order effect in $1/V$ with the unknown constant c_4 appears with a different coefficient from the two-point case (39) and (51), both χ_t and c_4 can be extracted by combining the two- and four-point correlators. Note that this calculation is free from short-distance singularities, because the operators are explicitly put apart from others. This is in contrast to the usual definition $\chi_t = (1/V) \int d^4x \langle \omega(x) \omega(0) \rangle$ (at a fixed θ).

C. Three-point correlation function

Topological susceptibility can be extracted also from *CP*-odd observables. The simplest case is given by a three-point function as

$$
\lim_{|x_i - x_j| \to \text{large}} \langle \omega(x_1)\omega(x_2)\omega(x_3) \rangle_Q
$$

$$
= \lim_{|x_i - x_j| \to \text{large}} \langle \omega(x_1)\omega(x_2)\omega(x_3) \rangle^{(3)} \frac{iQ}{2\chi_t^2 V^2} + O(V^{-3})
$$

$$
= -\lim_{|x_i - x_j| \to \text{large}} \langle \omega(x_1)\omega(x_2)\omega(x_3)Q^3 \rangle \frac{Q}{2\chi_t^2 V^2} + O(V^{-3})
$$

$$
= -3\chi_t \frac{Q}{V^2}\left[1 + \frac{7c_4}{6\chi_t^2 V} - \frac{Q^2}{3\chi_t V} \right] + O(V^{-4}).
$$
(63)

As in the cases of two- and four-point functions we may rewrite the above result in terms of the fermionic quantities,

$$
\lim_{|x_i - x_j| \to \text{large}} \langle mP(x_1)mP(x_2)mP(x_3) \rangle_Q
$$

$$
= \lim_{|x_i - x_j| \to \text{large}} \langle mP(x_1)mP(x_2)mP(x_3) \rangle^{\text{disc}}_Q
$$

$$
= \lim_{|x_i - x_j| \to \text{large}} \langle \omega(x_1)\omega(x_2)\omega(x_3) \rangle_Q
$$

$$
= -3\chi_t \frac{Q}{V^2}\left[1 + \frac{7c_4}{6\chi_t^2 V} - \frac{Q^2}{3\chi_t V} \right] + O(V^{-4}).
$$
(64)

As expected, the three-point function is useful only when the net topological charge is nonzero.

IV. *CP*-ODD ELECTROMAGNETIC FORM FACTOR

The three-point function considered above is an example of a *CP*-odd observable. In our formulation, as the formula (29) implies, the *CP*-odd observable (or its first derivative with respect to θ) can be calculated in a (nonzero) fixed topological sector. Another interesting example of this class is the neutron electric dipole moment.

The *CP*-odd electromagnetic form factor $F_3(q^2)$ is related to the neutron electric dipole moment d_N as

$$
d_N = \lim_{q^2 \to 0} \frac{F_3(q^2)}{2m_N},
$$
(65)

where q is a momentum transfer. It has been shown in [21] that $F_3(q^2)$ can be extracted from the correlation functions $\langle \bar{N}(p)J_\mu^{\text{EM}}(q)N(p')Q \rangle$ and $\langle \bar{N}(p)N(p)Q \rangle$, where $N(p)$ is a neutron interpolating field and J_μ^{EM} is the electromagnetic current. The momentum transfer is denoted by $q = p - p'$.

Once χ_t is extracted from the methods explained in the previous section, these neutron correlators can be extracted at a fixed topological charge using (29),

$$
\langle \bar{N}(p)J_\mu^{\text{EM}}(q)N(p') \rangle^{\text{odd}}_Q = \langle \bar{N}(p)J_\mu^{\text{EM}}(q)N(p')Q \rangle \frac{Q}{\chi_t V}
$$

$$
+ O(V^{-2}),
$$
(66)

$$
\langle \bar{N}(p)N(p) \rangle^{\text{odd}}_Q = \langle \bar{N}(p)N(p)Q \rangle \frac{Q}{\chi_t V} + O(V^{-2}),
$$
(67)

where the superscript "odd" means that a *CP*-odd part of the correlation function is considered.

V. CONCLUSIONS AND DISCUSSIONS

In this paper, we have derived general formulas which express arbitrary correlation functions at a fixed topological charge Q in terms of the same correlation function (and its derivatives) in the θ vacuum. As expected from the intuitive argument of local topological excitations, the difference between the fixed Q vacuum and the fixed θ vacuum disappears in the large volume limit as $1/V$. The relation is established only using fundamental properties of the quantum field theory, such as the cluster decomposition principle.

These formulas open a new possibility to calculate physical quantities in the lattice QCD simulations at a fixed topological charge. This will become unavoidable as the continuum limit is approached, irrespective of the lattice fermion formulation one employs, as far as the algorithm is based on the continuous evolution of the gauge field. (A proposal to avoid this limitation has recently been proposed [22]. Its numerical feasibility is yet to be investigated.)

For the correlators of the local topological charge operator, the $1/V$ expansion is worked out for two-, three-, and four-point functions to the second nontrivial order. The local topological charge operator may either be a bosonic one or a fermionic singlet pseudoscalar operator. At the leading nontrivial order the topological susceptibility χ_t appears as an expansion parameter, and a higher order parameter c_4 appears at the second order. In principle, these parameters can be determined by the lattice data. The different correlators and different V and Q may be used to check the results. This method is free from short-distance singularities, since the local topological charge operators are put apart from others and no contact term appears. Numerical calculation is in progress by the JLQCD Collaboration on the gauge configurations generated with a dynamical overlap fermion [5–8]. Once these parameters are numerically obtained, they can be used as input parameters for other physical observables.

The limitation of the formulas comes from the use of the saddle point expansion. It requires that the volume is large enough, $\chi_t V \gg 1$, that the local topological fluctuation is, in fact, active. It corresponds to the condition $\langle 0|Q^2|0 \rangle \gg 1$ for that volume. In addition, in order that the saddle point $\theta_c \simeq Q/(\chi_t V)$ can be expanded around $\theta = 0$, the (fixed) topological charge $|Q|$ must be much smaller than

$\chi_t V = \langle 0|Q^2|0\rangle$. Since χ_t is estimated in ChPT as $\chi_t = m\Sigma/N_f$ for N_f flavors of sea quarks, the condition is $|Q| \ll m\Sigma V$. This means that the system must be well separated from the ϵ regime ($m\Sigma V \lesssim 1$). This makes sense, because in the ϵ regime the physical quantities have substantial dependence on the topological charge and cannot be simply expressed by the saddle point expansion.

Our general formulas can also be applied to other observables, such as masses, decay constants, and matrix elements. Although the knowledge of the θ dependence of the observables is needed, only a few derivatives with respect to θ are sufficient for small θ, which is physically most relevant. Using the systematic $1/V$ expansion, one can, in principle, extract those derivatives to arbitrary finite order by looking at the Q dependence. Combining them with $\chi_t, c_4, \ldots$, the physical observables in the small θ vacuum can be reconstructed. This is not surprising, because if we were able to determine all the coefficients in $E(\theta)$, we could compute observables in the θ vacuum by a reweighting method. The point of our work is to present a practically feasible strategy in which the computational effort is drastically reduced. For the quantities well described by ChPT, estimation of the θ dependence based on the chiral Lagrangian is possible. Some results at the leading order were obtained in [12], and we are extending them to the next-to-leading order. This can also be used as an independent consistency check.

Once χ_t is extracted, we can calculate the first derivative of the *CP*-odd quantities from simulations at a fixed nonzero topological charge using (29). The most interesting such quantity in the context of lattice QCD calculation is the neutron electric dipole moment. For this quantity, the calculation of the *CP*-odd form factor in the fixed nonzero topological charge suffices to predict the physical result in the θ vacuum.

APPENDIX A: COMPARISON OF THE SADDLE POINT EXPANSION WITH AN EXACT θ INTEGRATION

In this appendix we demonstrate that the saddle point expansion reproduces the results from the exact θ integration, by considering a simple model for $E(\theta)$.

We consider the following form of the θ dependence:

$$E(\theta) = \chi_t[1 - \cos\theta]. \tag{A1}$$

The partition function Z_Q can be exactly calculated as

$$Z_Q = e^{-V\chi_t}I_Q(V\chi_t), \tag{A2}$$

where I_Q is the modified Bessel function. If the form of $G(\theta)$ is given, G_Q can also be calculated exactly. For example, let us consider the case that $G(\theta) = \langle\theta|Q|\theta\rangle$ or $\langle\theta|Q^2|\theta\rangle$. From $\langle\theta|Q|\theta\rangle = -iVdE/d\theta = -iV\chi_t\sin\theta$, we have

$$\langle Q\rangle_Q = \frac{-i}{Z_Q}\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}V\chi_t\sin\theta e^{-VE(\theta)+i\theta Q}$$
$$= V\chi_t\frac{I_{Q-1}(V\chi_t) - I_{Q+1}(V\chi_t)}{2I_Q(V\chi_t)}. \tag{A3}$$

Using a formula for the Bessel function $I_{n-1}(z) - I_{n+1}(z) = (2n/z)I_n(z)$, the correct result $\langle Q\rangle_Q = Q$ is reproduced. Similarly, using

$$\langle\theta|Q^2|\theta\rangle = \frac{d^2}{d\theta^2}\log Z(\theta) + \langle\theta|Q|\theta\rangle^2$$
$$= V\chi_t\cos\theta - (V\chi_t\sin\theta)^2, \tag{A4}$$

we obtain an expression

$$\langle Q^2\rangle_Q = \frac{z[I_{Q+1}(V\chi_t) + I_{Q-1}(V\chi_t)] + (z^2/2)[I_{Q+2}(V\chi_t) + I_{Q-2}(V\chi_t) - 2I_Q(V\chi_t)]}{2I_Q(V\chi_t)}, \tag{A5}$$

which leads to the correct result $\langle Q^2\rangle_Q = Q^2$.

We now consider a general $G(\theta)$. We will calculate G_Q, using the expansion of $G(\theta)$,

$$G_Q = G(0) + \sum_{n=1}^{\infty}\frac{G^{(n)}}{n!}\langle\theta^n\rangle, \tag{A6}$$

where

$$\langle\theta^n\rangle_Q = \frac{1}{Z_Q}\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}Z(\theta)e^{i\theta Q}\theta^n. \tag{A7}$$

This expansion can be evaluated using the connected part

$$\langle(i\theta)^n\rangle_{Q,c} = \frac{d^n}{dQ^n}\log Z_Q \tag{A8}$$

and the formulas

$$\langle X \rangle = \langle X \rangle_c, \tag{A9}$$

$$\langle X^2 \rangle = \langle X^2 \rangle_c + \langle X \rangle^2, \tag{A10}$$

$$\langle X^3 \rangle = \langle X^3 \rangle_c + 3\langle X^2 \rangle_c \langle X \rangle + \langle X \rangle^3, \tag{A11}$$

$$\langle X^4 \rangle = \langle X^4 \rangle_c + 4\langle X^3 \rangle_c \langle X \rangle + 3(\langle X^2 \rangle_c)^2 + 6\langle X^2 \rangle_c \langle X \rangle^2 + \langle X \rangle^4, \tag{A12}$$

with $X = \theta$ in our case. We evaluate the Q derivatives in the large V limit, using the asymptotic expansion of the Bessel function

$$I_Q(z) \simeq e^z \frac{1}{\sqrt{2\pi Z}} \sum_{n=0}^{\infty} (-1)^n (Q, n) \frac{1}{(2z)^n} + O(e^{-z}), \tag{A13}$$

where $z = \chi_t V$ and

$$(Q, n) = \frac{(4Q^2 - 1^2)(4Q^2 - 3^2) \cdots (4Q^2 - (2n-1)^2)}{n! 2^{2n}},$$
$$(Q, 0) = 1. \tag{A14}$$

Using these, the partition function is written as

$$Z_Q \simeq \frac{1}{\sqrt{2\pi z}} \left[1 - \frac{(Q, 1)}{2z} + \frac{(Q, 2)}{(2z)^2} + \cdots \right] \tag{A15}$$

and we obtain, ignoring $O(V^{-3})$ contributions,

$$\log Z_Q = -\log \sqrt{2\pi z} - \frac{1}{2z} \left[(Q, 1) + \frac{(Q, 1)^2}{2(2z)} - \frac{(Q, 2)}{2z} \right]$$
$$= -\log \sqrt{2\pi z} - \frac{1}{2z} \left(Q^2 - \frac{1}{4} \right) \left(1 + \frac{1}{2z} \right), \tag{A16}$$

from which

$$\frac{d}{dQ} \log Z_Q = -\frac{Q}{z} \left(1 + \frac{1}{2z} \right), \tag{A17}$$

$$\frac{d^2}{dQ^2} \log Z_Q = -\frac{1}{z} \left(1 + \frac{1}{2z} \right), \tag{A18}$$

$$\frac{d^n}{dQ^n} \log Z_Q = 0, \qquad n = 3, 4, 5, \cdots. \tag{A19}$$

Therefore,

$$\langle \theta \rangle_Q = i \frac{Q}{z} \left(1 + \frac{1}{2z} \right), \tag{A20}$$

$$\langle \theta^2 \rangle_Q = \frac{1}{z} \left(1 + \frac{1}{2z} \right) - \frac{Q^2}{z^2} + O(z^{-3}), \tag{A21}$$

$$\langle \theta^3 \rangle_Q = i \frac{3Q}{z^2} + O(z^{-3}), \tag{A22}$$

$$\langle \theta^4 \rangle_Q = \frac{3}{z^2} + O(z^{-3}). \tag{A23}$$

Collecting these, the final result becomes

$$G_Q = G(0) + G^{(2)}(0) \frac{1}{2z} \left(1 + \frac{1}{2z} - \frac{Q^2}{z} \right) + G^{(4)}(0) \frac{1}{8z^2}$$
$$+ G^{(1)}(0) i \frac{Q}{z} \left(1 + \frac{1}{2z} \right) + G^{(3)}(0) i \frac{Q}{2z^2}. \tag{A24}$$

Noticing that $c_4 = -\chi_t$ for the present case, this result completely agrees with the previous result (27) within the $O(V^{-3})$ errors. This demonstrates that the saddle point expansion reproduces correct results, up to exponentially small corrections.

The leading order of the chiral perturbation theory gives

$$E(\theta) = N_f^2 \chi_t [1 - \cos(\theta/N_f)]. \tag{A25}$$

In this case, we can extend the integration range to $-N_f \pi < \theta < N_f \pi$ by ignoring exponentially small contributions. After performing θ integration exactly, we obtain

$$Z_Q = e^{-z} I_{\hat{Q}}(z) + O(e^{-z[1-\cos(\pi/N_f)]}) \tag{A26}$$

where $z = V N_f^2 \chi_t$ and $\hat{Q} = N_f^2 Q$. Noticing that $c_4 = -\chi_t/N_f^2$ in this case, it is easy to see that the saddle point expansion agrees with exact results order by order in the $1/V$ expansion, as long as exponentially small corrections are ignored.

APPENDIX B: CONTRIBUTIONS AT V^{-3}

1. *CP*-even contributions

For $\theta_c = O(V^{-1})$, *CP*-even contributions become

$$G_Q^{\text{even}} = G + G^{(2)} \frac{\theta_c^2}{2} + G^{(2)} \frac{1}{2x} \left(1 - \frac{E^{(4)}V}{2x^2} - \frac{E^{(6)}V}{8x^3} + \frac{2(E^{(4)}V)^2}{3x^4} + \frac{5(E^{(3)}V)^2}{4x^3} \right) + G^{(4)} \frac{\theta_c^2}{4x}$$
$$+ G^{(4)} \frac{1}{4!} \left(\frac{3}{x^2} - \frac{4E^{(4)}V}{x^4} \right) + G^{(6)} \frac{15}{6! x^3}$$
$$- G^{(2)} \theta_c \frac{E^{(3)}V}{2x^2} + O(V^{-4}). \tag{B1}$$

Using the large separation limit $G = G^{(2)} = 0$, $G^{(4)} = 24\chi_t^4$, and $G^{(6)} = 480\chi_t^3 c_4$ for $G = \langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle$, we obtain

$$\langle \omega(x_1)\omega(x_2)\omega(x_3)\omega(x_4) \rangle_Q \rightarrow \frac{3\chi_t^2}{V^2} \left[1 + \frac{2}{\chi_t^2 V} (c_4 - Q^2 \chi_t) \right] + O(V^{-4}). \tag{B2}$$

2. *CP*-odd contributions

For $\theta_c = O(V^{-1})$, *CP*-odd contributions become

$$
\begin{aligned}
G_Q^{\text{odd}} = {} & G^{(1)}\theta_c + G^{(3)}\frac{\theta_c^3}{3!} + G^{(3)}\frac{\theta_c}{2x}\left(1 - \frac{E^{(4)}V}{2x^2}\right) \\
& + G^{(5)}\frac{3\theta_c}{4!x^2} - G^{(1)}\left[\frac{E^{(3)}V}{2x^2}\left(1 - \frac{4E^{(4)}V}{3x^2}\right) + \frac{E^5 V}{8x^3}\right] \\
& - G^{(3)}\frac{5E^{(3)}V}{12x^3}.
\end{aligned}
\tag{B3}
$$

Using the large separation limit $G^{(1)} = 0$, $G^{(3)} = i6\chi_t^3$, and $G^{(5)} = i60\chi_t^2 c_4$ for $G = \langle\omega(x_1)\omega(x_2)\omega(x_3)\rangle$, we obtain

$$
\langle\omega(x_1)\omega(x_2)\omega(x_3)\rangle_Q \rightarrow -\frac{Q}{V^2}\left[3\chi_t + \frac{7c_4}{2\chi_t V} - \frac{Q^2}{V}\right].
\tag{B4}
$$

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