

## $\theta$ vacuum physics from QCD at fixed topology

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We propose a method to obtain physical quantities in the  $\theta$  vacuum from those at fixed topology, which are different by finite size effects. Extending the work by Brower *et al.*, we derive the formula to estimate these finite size corrections for arbitrary correlators in terms of the topological susceptibility and the  $\theta$  dependence. Applying this formula, we show that topological susceptibility can be measured through two-point functions of pseudoscalar operator.

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## 1. Introduction

In Quantum Chromodynamics (QCD), the ground state must be the  $\theta$  vacuum in order to ensure the cluster decomposition property of physical observables. However, in unquenched lattice QCD simulations by Hybrid Monte Carlo algorithm [1], the correct sampling of topological charge will become increasingly more difficult [2, 3]. In view of this situation, one promising approach is to fix the topology during the Hybrid Monte Carlo simulation and try to extract physics from the simulations at a fixed topological charge  $Q$ . It is known that the fixed  $Q$  effect is a finite size effect which vanishes in the infinite volume limit. In this report, we give a theoretical basis for estimating the finite size effect in order to extract physics in the  $\theta$  vacuum from QCD at fixed topology [4], by extending the work by Brower et al. [5]. We derive a general formula to estimate this relation. Furthermore, using our formula, we propose a method to measure the topological susceptibility at fixed topology. The numerical study is given in a separate reports [6, 7].

## 2. General formula

Consider the partition function in the  $\theta$  vacuum defined by

$$Z(\theta) \equiv \langle \theta | \theta \rangle = \exp[-VE(\theta)], \quad (2.1)$$

where  $E(\theta)$  is the vacuum energy density. The topological susceptibility  $\chi_t$  at  $\theta = 0$  is defined by

$$\chi_t = \frac{\langle 0 | Q^2 | 0 \rangle}{V} = \left. \frac{d^2 E(\theta)}{d\theta^2} \right|_{\theta=0}. \quad (2.2)$$

Since  $\chi_t \geq 0$  by definition,  $\theta = 0$  is a local minimum of  $E(\theta)$ . Moreover, Vafa and Witten proved that  $Z(0) > Z(\theta)$  [8], so that  $\theta = 0$  is the global minimum of the function  $E(\theta)$ . Assuming analyticity of  $E(\theta)$  near  $\theta = 0$ , we can expand  $E(\theta)$  as

$$E(\theta) = \sum_{n=1}^{\infty} \frac{c_{2n}}{(2n)!} \theta^{2n} = \frac{\chi_t}{2} \theta^2 + O(\theta^4). \quad (2.3)$$

The partition function at a fixed topological charge  $Q$  is a Fourier transformation of  $Z(\theta)$

$$Z_Q = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta Z(\theta) \exp(i\theta Q) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \exp(-VF(\theta)), \quad (2.4)$$

where  $F(\theta) \equiv E(\theta) - i\theta Q/V$ . For a large enough volume, we can evaluate the  $\theta$  integral in (2.4) by the saddle point expansion. The saddle point  $\theta_c$  is given by

$$\theta_c = i \frac{Q}{\chi_t V} (1 + O(\delta^2)), \quad (2.5)$$

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

$$F(\theta) = F(\theta_c) + \frac{E^{(2)}(\theta_c)}{2} (\theta - \theta_c)^2 + \sum_{n=3}^{\infty} \frac{E^{(n)}(\theta_c)}{n!} (\theta - \theta_c)^n, \quad (2.6)$$

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

$$VF(\theta_c) = \frac{Q^2}{2\chi_t V}(1 + O(\delta^2)), \quad E^{(2)}(\theta_c) = \chi_t(1 + O(\delta^2)), \quad (2.7)$$

$$E^{(2n)}(\theta_c) = c_{2n}(1 + O(\delta^2)), \quad E^{(2n-1)}(\theta_c) = \theta_c c_{2n}(1 + O(\delta^2)). \quad (2.8)$$

By a change of variable  $s = \sqrt{E^{(2)}V}(\theta - \theta_c)$  we can rewrite the integral as

$$Z_Q = \frac{e^{-VF(\theta_c)}}{2\pi\sqrt{E^{(2)}V}} \int_{-\sqrt{E^{(2)}V}(\pi-\theta_c)}^{\sqrt{E^{(2)}V}(\pi-\theta_c)} ds \exp\left[-\frac{s^2}{2} - \sum_{n=3} \frac{E^{(n)}V}{n!} \left(\frac{s}{\sqrt{E^{(2)}V}}\right)^n\right] \quad (2.9)$$

Neglecting exponentially suppressed terms and expanding in powers of  $1/V$ , we obtain

$$Z_Q = \frac{1}{\sqrt{2\pi\chi_t V}} \exp\left[-\frac{Q^2}{2\chi_t V}\right] \left[1 - \frac{c_4}{8V\chi_t^2} + O\left(\frac{1}{V^2}, \delta^2\right)\right]. \quad (2.10)$$

This shows that, as long as  $\delta \ll 1$  (equivalently,  $Q \ll \chi_t V$ ), the distribution of  $Q$  becomes the Gaussian distribution. Similarly, consider an arbitrary correlation function in  $\theta$  vacuum and at fixed topological charge  $Q$  are defined as

$$G(\theta) = \langle \theta | O_1 O_2 \cdots O_n | \theta \rangle, \quad G_Q = \frac{1}{Z_Q} \frac{1}{2\pi} \int d\theta Z(\theta) G(\theta) \exp(i\theta Q). \quad (2.11)$$

Using the saddle point expansion as before, if  $G$  is CP-even, we can show

$$G_Q^{\text{even}} = G(0) + G^{(2)}(0) \frac{1}{2\chi_t V} \left[1 - \frac{Q^2}{\chi_t V} - \frac{c_4}{2\chi_t^2 V}\right] + G^{(4)}(0) \frac{1}{8\chi_t^2 V^2} + O(V^{-3}), \quad (2.12)$$

where  $G^{(n)}(0)$  stands for the  $n$ -th derivative of  $G$  with respect to  $\theta$ . If  $G$  is CP-odd, we have

$$G_Q^{\text{odd}} = G^{(1)}(0) \frac{iQ}{\chi_t V} \left(1 - \frac{c_4}{2\chi_t^2 V}\right) + G^{(3)}(0) \frac{iQ}{2\chi_t^2 V^2} + O(V^{-3}). \quad (2.13)$$

The formula (2.12) provides an estimate of the finite size effect due to the fixed topological charge. The leading correction is of order  $O(1/V)$ . It should be also noted that the other formula (2.13) suggests that it is possible to extract the  $\theta$  dependence of CP-odd observables, such as the neutron electric dipole moment by measuring the observable at a fixed non-zero topological charge, once the topological susceptibility  $\chi_t$  is obtained.

### 3. Topological susceptibility

There are two reasons for measuring topological susceptibility. The primary reason is to study whether the local topological fluctuation is sufficiently created in unquenched QCD simulations. In conventional quenched QCD simulations, the topology change during Monte Carlo updates is triggered by the formation of dislocations which grows into local topological fluctuation with positive or negative topological charge. This is a topology non-conserving processes through lattice artifact. On the other hand, in unquenched simulations such process is highly suppressed towards

continuum and chiral limit. In particular, unquenched simulations by the JLQCD collaboration explicitly prohibits such processes by introducing extra Wilson fermions [9]. Then, the main source of the local topological fluctuation is achieved through the pair creation of local fluctuation of positive and negative topological charge densities, just as in the continuum theory. Therefore, the measurement of the topological susceptibility is a crucial test of the thermal equilibrium in local topological fluctuation. The secondary reason is that the topological susceptibility is the key quantity to estimate the finite size effects at fixed topology as was shown in the previous section.

Recently, there are several proposals for the field theoretical definitions of the topological susceptibility, which are free from ambiguities. The first one is given by Giusti et al. [10] in which they define the topological susceptibility by the integration of disconnected flavor-singlet pseudoscalar correlator. The second one is a UV divergence free definition by Luscher [11] in terms of  $n$ -point function of flavor non-singlet scalar and pseudoscalar correlator. The third one is proposed in the study of Schwinger model [12]. They extracted the topological susceptibility from the asymptotical value of the singlet pseudoscalar correlator up to  $1/V$  correction as

$$\lim_{x \rightarrow \infty} \langle mP(x)mP(0) \rangle_{Q,V} = \frac{1}{V} \left( \frac{Q^2}{V} - \chi_t \right) + \mathcal{O}(V^{-2}). \quad (3.1)$$

Although the intuitive picture for this relation was given in Ref. [12], the field theoretical proof based was given only recently, which will be explained in the next subsection.

### 3.1 Field theoretical proof of the formula for the topological susceptibility

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. (2.12) gives

$$\begin{aligned} \langle \omega(x)\omega(0) \rangle_Q &= \langle \omega(x)\omega(0) \rangle + \langle \omega(x)\omega(0) \rangle^{(2)} \frac{1}{2V\chi_t} \left( 1 - \frac{Q^2}{V\chi_t} - \frac{c_4}{2\chi_t^2 V} \right) \\ &\quad + \langle \omega(x)\omega(0) \rangle^{(4)} \frac{1}{8\chi_t^2 V^2} + \mathcal{O}(V^{-3}), \end{aligned} \quad (3.2)$$

where  $\langle O \rangle^{(n)}$  is the  $n$ -th derivative of  $\langle O \rangle$  with respect to  $\theta$ . In the large separation limit  $|x| \rightarrow \infty$ , the CP invariance at  $\theta = 0$  and the clustering property at a fixed  $\theta$  gives

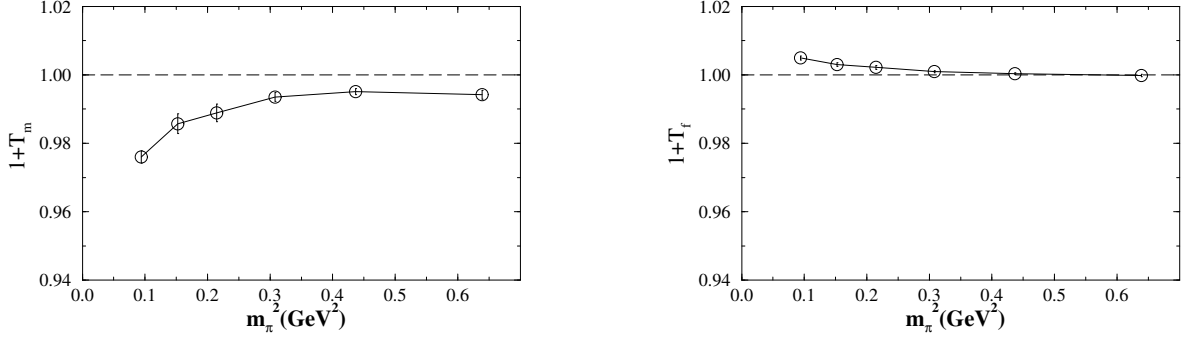
$$\lim_{|x| \rightarrow \text{large}} \langle \omega(x)\omega(0) \rangle_Q = \frac{1}{V} \left( \frac{Q^2}{V} - \chi_t - \frac{c_4}{2\chi_t V} \right) + \mathcal{O}(V^{-3}) + \mathcal{O}(e^{-m_{\eta'}|x|}), \quad (3.3)$$

where the flavor singlet pseudo-scalar meson mass,  $m_{\eta'}$ , is the lightest mass of possible intermediate states.

Physical quantities such as the topological susceptibility  $\chi_t$  can be obtained through (3.3). In practice, this formula will be used for a finite separation  $x$  instead of  $|x| \rightarrow \infty$ . The clustering property in the  $\theta$  vacuum receives a correction of order of  $e^{-m_{\eta'}|x|}$ , which vanishes quickly because the flavor singlet meson  $\eta'$  acquires a large mass due to the axial anomaly of QCD.

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) Ward-Takahashi (WT) identities for an arbitrary operator  $O$ :

$$\langle \partial_\mu A_\mu(x)O - 2mP(x)O + 2\omega(x)O + \delta_x O \rangle = 0, \quad (3.4)$$



**Figure 1:** The finite size effects  $1 + T_m$  (left panel) and  $1 + T_f$  (right panel) from fixed topology at  $Q = 0$  with  $L = 2$  fm. The pion masses correspond to those in the dynamical simulation by the JLQCD collaboration.

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 pseudo-scalar density, respectively, and  $\delta_x O$  denotes a axial rotation of the operator  $O$  at  $x$ . Combining WT identities for  $O = 2mP(0)$  and  $O = 2\omega(x)$  Combining these we finally obtain

$$\lim_{|x| \rightarrow \text{large}} \langle mP(x)mP(0) \rangle_Q = \frac{1}{V} \left( \frac{Q^2}{V} - \chi_t - \frac{c_4}{2\chi_t V} \right) + O(e^{-m_{\eta'}|x|}). \quad (3.5)$$

In fact, using this formula one can determine the topological susceptibility from the nonzero asymptotic value of the singlet pseudoscalar correlator [6, 7].

#### 4. Application to physics

One can estimate the finite size corrections for the pionic quantities with the help of Chiral Perturbation Theory (ChPT). Using the next-to-leading order ChPT formula,  $\theta$  dependence of the the pion mass and the decay constant for two-flavor QCD is

$$m_\pi^2(\theta)|_{rmNLO} = m_\pi^2(\theta) \left[ 1 + \left( \frac{m_\pi(\theta)}{4\pi f} \right)^2 \left( \ln \left( \frac{m_\pi(\theta)}{m_\pi^{\text{phys}}} \right)^2 - \bar{l}_3^{\text{phys}} \right) \right], \quad (4.1)$$

$$f_\pi(\theta)|_{rmNLO} = f \left[ 1 - 2 \left( \frac{m_\pi(\theta)}{4\pi f} \right)^2 \left( \ln \left( \frac{m_\pi(\theta)}{m_\pi^{\text{phys}}} \right)^2 - \bar{l}_4^{\text{phys}} \right) \right], \quad (4.2)$$

where  $m_\pi^2(\theta) \equiv 2B_0 m_q \cos \left( \frac{\theta}{N_f} \right)$ , and  $\bar{l}_3, \bar{l}_4$  are the low energy constants which can be estimated as  $\bar{l}_3^{\text{phys}} = 2.9 \pm 2.4$ , and  $\bar{l}_4^{\text{phys}} = 4.4 \pm 0.2$  [17]. Fig. 1 shows the finite size effects  $1 + T_m \equiv m_\pi^{Q=0}/m_\pi$  and  $1 + T_f \equiv f_\pi^{Q=0}/f_\pi$  at  $L = 2$  fm using the NLO ChPT. The pion masses correspond to those in the dynamical simulation by the JLQCD collaboration [18]. The topological susceptibility  $\chi_t$  is

extracted from the singlet pseudoscalar correlator as explained in the previous section. It is found that finite size effect for the pion mass ranges from 0.5 to 2.5 %, whereas that for the pion decay constant is well below 0.5%. These finite size correction from fixing the topology is correctly taken into account in the spectrum study [18]. In general, for quantities which has a non-vanishing chiral limit,  $\theta$  or  $Q$  dependence correction only comes through  $m_\pi(\theta)$  as sub-leading corrections. Therefore, pion receives the largest finite size correction. This means that if the finite size effect of the pion mass is under control, other hadronic quantities are safe.

#### 4.1 Nongaussianity of the topological charge distribution

Recently deviation of the topological charge distribution from Gaussian is observed for pure Yang-Mills gauge theory [13, 14, 15, 16]. In principle, we can also measure the deviation from the Gaussian ( $c_4$  coefficient) by combining the 2-, 3-, 4-point functions of the topological charge density given as follows

$$\lim_{|x| \rightarrow \text{large}} \langle \omega(x) \omega(0) \rangle_Q = -\frac{\chi_t}{V^2} \left[ 1 - \frac{1}{2\chi_t^2 V} (c_4 - 2\chi_t Q^2) \right] + O(V^{-3}) \quad (4.3)$$

$$\lim_{|x_i - x_j| \rightarrow \text{large}} \langle \omega(x_1) \omega(x_2) \omega(x_3) \rangle_Q = -3\chi_t \frac{Q}{V^2} \left[ 1 + \frac{7}{6\chi_t^2 V} (c_4 - \frac{2}{7}\chi_t Q^2) \right] + O(V^{-4}) \quad (4.4)$$

$$\lim_{|x_i - x_j| \rightarrow \text{large}} \langle \omega(x_1) \omega(x_2) \omega(x_3) \omega(x_4) \rangle_Q = 3\frac{\chi_t^2}{V^2} \left[ 1 + \frac{1}{\chi_t^2 V} (c_4 - \chi_t Q^2) \right]^2 + O(V^{-4}). \quad (4.5)$$

### 5. Summary

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  $\theta$  vacuum. The difference between the fixed  $Q$  vacuum and the fixed  $\theta$  vacuum can be shown to disappear in the large volume limit as  $1/V$  only using fundamental properties of the quantum field theory.

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.

Applying the formula for  $n$ -point functions of the topological charge density  $\omega$ , we have shown that the topological susceptibility  $\chi_t$  and  $c_4$  appear at the first and second order corrections, respectively. In principle, these parameters can be determined by the lattice data. Our 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 dynamical overlap fermion [19, 20, 21, 22]. Once these parameters are numerically obtained, they can be used as input parameters for other physical observables, such as weak matrix elements such as  $B_K$  [23], pion form factor [24], the neutron electric dipole moment, and so on.

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