

## $\theta = \pi$ in $SU(N)/\mathbb{Z}_N$ gauge theories

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**ABSTRACT:** In  $SU(N)$  gauge theory, it is argued recently that there exists a “mixed anomaly” between the CP symmetry and the 1-form  $\mathbb{Z}_N$  symmetry at  $\theta = \pi$ , and the anomaly matching requires CP to be spontaneously broken at  $\theta = \pi$  if the system is in the confining phase. In this paper, we elaborate on this discussion by examining the large volume behavior of the partition functions of the  $SU(N)/\mathbb{Z}_N$  theory on  $T^4$  à la ’t Hooft. The periodicity of the partition function in  $\theta$ , which is not  $2\pi$  due to fractional instanton numbers, suggests the presence of a phase transition at  $\theta = \pi$ . We propose lattice simulations to study the distribution of the instanton number in  $SU(N)/\mathbb{Z}_N$  theories. A characteristic shape of the distribution is predicted when the system is in the confining phase. The measurements of the distribution may be useful in understanding the phase structure of the theory.

**KEYWORDS:** Discrete Symmetries, Lattice Quantum Field Theory, Wilson, ’t Hooft and Polyakov loops, Confinement

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## 1 Motivation

The  $\theta$ -term in 4D gauge theories specifies how to sum up topologically inequivalent sectors in the path integral. In the real world, the value of the  $\theta$  parameter in QCD is physical and known to be unnaturally small if the up-quark mass is non-vanishing. Unlike other parameters in the Lagrangian, the  $\theta$  parameter only shows up at the non-perturbative level. The reaction of the theory to the change of the  $\theta$  parameter gives us quite important information on the vacuum structure of the theory.

The theory at  $\theta = \pi$  is somewhat interesting. It is the point where the Lagrangian has CP invariance (up to  $2\pi$  shift of  $\theta$ ), as well as at  $\theta = 0$ . A non-trivial phenomenon at  $\theta = \pi$  has been found in 4D bosonic pure Yang-Mills theory in the large  $N$  limit [1, 2]. It is shown in [1, 2] that the vacuum energy of the theory depends on  $\theta$  as

$$F(\theta) = C \min_k (\theta + 2\pi k)^2 + O(1/N) \tag{1.1}$$

with a constant  $C$ . At  $\theta = \pi$ , this function has a cusp. This shows that the expectation value  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle$  has a discontinuity there, indicating the spontaneous CP violation. One may investigate the same kind of phenomenon in a more rigorous way for  $\mathcal{N} = 1$  super Yang-Mills theory with gauge group SU( $N$ ) when a small gaugino mass  $m$  is added which breaks supersymmetry [4–8]. The following effective potential

$$F(\theta) = -2m\mu^3 e^{-8\pi^2/(g(\mu)^2 N) + i\theta/N} + \text{c.c.}, \tag{1.2}$$

is induced, where  $\mu$  is a renormalization scale. When  $\theta = \pm\pi$ , a pair of vacua degenerate. The potential (1.2) implies that the expectation values  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle$  at  $\theta = \pm\pi$  are nonzero and have opposite signs with each other. Although the limit  $m \rightarrow \infty$  is hard to study, this example indicates that the spontaneous CP violation may occur also for finite  $N$  gauge

theories. Indeed, 't Hooft has argued that there must be a phase transition at some value of  $\theta$  (likely to be at  $\theta = \pi$ ) if electric confinement takes place for all values of  $\theta$  [9]. The possibility of a transition to the oblique confinement phase near  $\theta \simeq \pi$  has been proposed in ref. [10]. See ref. [3] for the discussion on spontaneous C and P violation at  $\theta = \pi$  in 2D  $\mathbb{C}\mathbb{P}^{N-1}$  models.

Recently, a renewed discussion has led to the conclusion that there must be spontaneous CP violation at  $\theta = \pi$  in bosonic  $SU(N)$  Yang-Mills theory in the confining phase [8]. The argument is based on the “anomaly matching” for the mixed anomaly between CP symmetry and the center symmetry. The latter is an example of the 1-form symmetry [11]. A background gauge field for the 1-form  $\mathbb{Z}_N$  symmetry breaks the  $2\pi$  periodicity for the  $\theta$  parameter, which makes it impossible to maintain the CP invariance at  $\theta = 0$  and  $\theta = \pi$  simultaneously. This anomaly should persist at any energy scale. In the infrared, assuming that the theory is in the confining phase, the low energy effective theory is trivial. However, the trivial theory cannot produce the mixed CP- $\mathbb{Z}_N$  anomaly, indicating that CP should be spontaneously broken in the  $SU(N)$  gauge theory, since the 1-form  $\mathbb{Z}_N$  symmetry is preserved in the confining phase. This anomaly matching argument has been applied to other theories in [12–15] for the discussion on their phase structure.

Motivated by the work in [8], we try to understand the spontaneous CP violation in  $SU(N)$  Yang-Mills theory on  $\mathbb{R}^4$  by studying the large volume limit of  $SU(N)/\mathbb{Z}_N$  Yang-Mills theory on  $T^4$ . The discussion is along the line of the argument of 't Hooft [9] where free energies of electric and magnetic line operators [16] are studied as functions of  $\theta$ . As discussed in [17–19], there are non-trivial bundles on  $T^4$  in  $SU(N)/\mathbb{Z}_N$  theory, realized by twisted boundary conditions. These topologically inequivalent bundles should be summed up in the path integral. Whereas in  $SU(N)$  theory, only the trivial topology, except for instantons, is allowed. This makes two theories,  $SU(N)$  and  $SU(N)/\mathbb{Z}_N$  theories, different from each other. However, in the confining phase where the correlation lengths between local operators are finite, local physics in the two theories should still be identical with each other when the volume of  $T^4$  is large enough. Instead, a difference of these theories can be found in the partition functions. In  $SU(N)/\mathbb{Z}_N$  theory on  $T^4$ , magnetic line operators are light in the confining phase since magnetic fluxes are screened. This means that the sectors with non-trivial bundles may contribute to the path integral even in the large volume limit. We find that these two facts, the same local physics and different partition functions, suggest the presence of a phase transition in  $SU(N)$  theory on  $\mathbb{R}^4$  at some value of  $\theta$ .

We find possible applications of our discussion to lattice gauge theory. By putting  $SU(N)/\mathbb{Z}_N$  theory on the lattice and by measuring the instanton numbers which can be fractional, one can extract information on the phase structure of  $SU(N)$  theory. We discuss what kinds of phenomena are anticipated, and also what are advantages to study  $SU(N)/\mathbb{Z}_N$  theory rather than  $SU(N)$  theory directly.

This paper is organized as follows. In section 2, we review  $SU(N)/\mathbb{Z}_N$  gauge theory on  $T^4$ , focusing on its global structures. The dynamical aspects of this theory are investigated in section 3 where we show a strong evidence of the existence of a first order phase transition with the spontaneous CP violation. In section 4, we argue possible implications for lattice simulation of  $SU(N)/\mathbb{Z}_N$  gauge theory on  $T^4$ .

## 2 $SU(N)/\mathbb{Z}_N$ gauge theory on $T^4$

In the following, we consider a gauge theory on  $T^4$  whose gauge group is  $G := SU(N)/\mathbb{Z}_N$ . This theory is locally equivalent to  $\tilde{G} := SU(N)$  theory. However, the global structure of the former theory is known to be much richer than that of the latter theory.

Let us recall the global formulation of a gauge theory on a general manifold  $M$  [20]. Let  $M = \bigcup_i U_i$  be an open covering of  $M$ . For each intersection  $U_{ij} := U_i \cap U_j$ , we define a transition function  $g_{ij}$  which takes its values in  $G$ . The transition functions must satisfy

$$g_{ij} = g_{ji}^{-1} \text{ on } U_{ij}, \quad g_{ij}g_{jk}g_{ki} = 1 \text{ on } U_{ijk}, \quad (2.1)$$

where  $U_{ijk} := U_i \cap U_j \cap U_k$ . A principal  $G$ -bundle is defined by gluing  $U_i \times G$  using  $g_{ij}$ . The gauge field is defined as a connection on this principal  $G$ -bundle.

To see the difference between  $G$  theory and  $\tilde{G}$  theory, we examine whether a given  $G$ -bundle can be regarded as a  $\tilde{G}$ -bundle. There is the canonical homomorphism

$$\pi : \tilde{G} \rightarrow G \quad (2.2)$$

whose kernel is  $\mathbb{Z}_N$ . For each element  $g \in G$ , one can choose an element  $\tilde{g} \in \tilde{G}$  such that  $\pi(\tilde{g}) = g$  holds. By this procedure, and assuming the continuity, the transition functions  $g_{ij}$  can be uplifted to functions  $\tilde{g}_{ij}$  which take their values in  $\tilde{G}$ . The functions  $\tilde{g}_{ij}$ , however, may not define transition functions for a principal  $\tilde{G}$ -bundle since the choice of  $\tilde{g} \in \tilde{G}$  for a given  $g \in G$  is not unique. In general, they satisfy

$$\tilde{g}_{ij}\tilde{g}_{jk}\tilde{g}_{ki} = C_{ijk} \in \mathbb{Z}_N \text{ on } U_{ijk}. \quad (2.3)$$

This is due to the fact that  $\pi(C_{ijk}) = 1$  holds.

There is a possibility that all  $C_{ijk}$  can be set to the identity by choosing a suitable  $\tilde{g}_{ij}$  for each  $g_{ij}$ . This corresponds to multiplying a suitable  $C_{ij} \in \mathbb{Z}_N$  to each  $g_{ij}$ . Then,  $C_{ijk}$  changes as

$$C_{ijk} \rightarrow C'_{ijk} := C_{ijk}C_{ij}^{-1}C_{jk}^{-1}C_{ki}^{-1}. \quad (2.4)$$

These two sets of the factors  $\{C_{ijk}\}$  and  $\{C'_{ijk}\}$  are regarded as equivalent since they are obtained from the same  $G$ -bundle. Therefore, each principal  $G$ -bundle is associated to a 2-cocycle on  $M$  whose values are in  $\mathbb{Z}_N$ . They are classified by the cohomology group  $H^2(M, \mathbb{Z}_N)$  [21].

Consider the case  $M = T^4$ . It is easy to show that

$$H^0(S^1, \mathbb{Z}_N) = H^1(S^1, \mathbb{Z}_N) = \mathbb{Z}_N \quad (2.5)$$

holds. By Künneth formula, one finds

$$H^2(T^4, \mathbb{Z}_N) = (\mathbb{Z}_N)^6. \quad (2.6)$$

This implies that there are  $N^6$  kinds of distinct  $G$ -bundles among which only one can be regarded as a  $\tilde{G}$ -bundle.

$G$ -bundles on  $T^4$  can be described more explicitly as follows [17–19]. The global structure of a  $G$ -bundle on  $T^4$  comes from a twisted boundary condition for the gauge field. Let us define coordinates  $x_\mu$  on  $T^4$  such that  $x_\mu = 0$  and  $x_\mu = a_\mu$  are identified. The gauge field at  $x_\mu = a_\mu$  is related to the one at  $x_\mu = 0$  by a gauge transformation as

$$A_\lambda(x_\mu = a_\mu) = \Omega_\mu A_\lambda(x_\mu = 0) \Omega_\mu^{-1} - i \Omega_\mu \partial_\lambda \Omega_\mu^{-1}. \tag{2.7}$$

The compatibility conditions for  $\Omega_\mu$  are

$$\Omega_\mu(x_\nu = a_\nu) \Omega_\nu(x_\mu = 0) = e^{2\pi i n_{\mu\nu}/N} \Omega_\nu(x_\mu = a_\mu) \Omega_\mu(x_\nu = 0), \tag{2.8}$$

where  $n_{\mu\nu}$  are integers modulo  $N$ . Note that  $n_{\mu\nu}$  is anti-symmetric. These integers label  $N^6$  distinct  $G$ -bundles.

The non-triviality of  $G$ -bundles appears in the values of the Pontryagin index. It is given by [18, 19]

$$P = \frac{1}{16\pi^2} \int d^4x F_{\mu\nu} \tilde{F}_{\mu\nu} = \nu + \left( \frac{N-1}{N} \right) \frac{n_{\mu\nu} \tilde{n}_{\mu\nu}}{4}, \tag{2.9}$$

where  $\nu$  is an integer and

$$\tilde{n}_{\mu\nu} := \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} n_{\rho\sigma}. \tag{2.10}$$

For example, for  $n_{12} = n_{34} = 1$  and zeros for other components, we have

$$P = \nu + \frac{N-1}{N}. \tag{2.11}$$

Therefore, the index is not an integer in general.

The Pontryagin index appears in the action of  $G$  theory as the  $\theta$ -term. The partition function  $Z_G(\theta, V)$  is given as

$$Z_G(\theta, V) = \sum_{n_{\mu\nu}, \nu} Z_G(n, \nu, V) e^{iP\theta} \tag{2.12}$$

where  $Z_G(n, \nu, V)$  is the path integral over the sector with fixed  $n_{\mu\nu}$  and  $\nu$ , in which the action does not contain the  $\theta$ -term. Since  $P$  takes fractional values (2.11),  $Z_G(\theta, V)$  has  $2N\pi$  periodicity. On the other hand, the partition function of  $\tilde{G}$  theory is

$$Z_{\tilde{G}}(\theta, V) = \sum_{\nu} Z_G(0, \nu, V) e^{i\nu\theta} \tag{2.13}$$

which has  $2\pi$  periodicity.

The integers  $n_{\mu\nu}$  have the following physical meaning. Suppose that  $\mu = 4$  corresponds to the time direction. Then  $n_{\mu\nu}$  can be decomposed into

$$k_i := n_{i4} \quad \text{and} \quad m_i := \frac{1}{2} \epsilon_{ijk} n_{jk}, \tag{2.14}$$

where  $i, j, k = 1, 2, 3$ . In the following, we denote the path integral with fixed  $k_i, m_i, \nu$  as  $Z_G(k, m, \nu, V)$ .

The 3-vector  $m_i$  is called the magnetic flux. This name is justified by observing that  $m_i$  changes by one if an 't Hooft line operator along the  $i$ -th direction is inserted. Then, one might expect that  $k_i$  would be interpreted as the electric flux. However, this turns out not to be the case. Instead, another 3-vector  $e_i$  which appears in the following expression [9]

$$e^{-VF_G(e,m,\theta,V)} = \frac{1}{N^3} \sum_{k,\nu} e^{-2\pi i k_i e_i / N + i\theta(\nu - k_i m_i / N)} Z_G(k, m, \nu, V), \quad (2.15)$$

is called the electric flux. This is because  $e_i$  changes by one if a Wilson line operator along the  $i$ -th direction is inserted. The quantity  $F_G(e, m, \theta, V)$  in the left-hand side is the free energy density for a sector with fixed  $e_i$  and  $m_i$ .

In the canonical formalism, the fluxes appear as follows [21]. The Hilbert space of  $G$  theory on  $T^4$  is the space of wave functions on the configuration space which is the space of connections on a  $G$ -bundle on the spatial manifold  $T^3$ . The  $G$ -bundles on  $T^3$  are classified by  $H^2(T^3, \mathbb{Z}_N) = (\mathbb{Z}_N)^3$ . They are labeled by the magnetic flux  $m_i$ . In defining the partition function on  $T^4$ , one may insert a twist in the time-direction. The twist is a gauge transformation which is specified by  $e_i$ .

### 3 Large volume limit

Local physical quantities, such as  $n$ -point functions of local operators, should become independent of the volume  $V$  of  $T^4$  when  $V$  is large enough. More precisely, if the theory under consideration has a mass gap  $\Delta > 0$ , then the volume-independence is expected when the size  $V^{1/4}$  of  $T^4$  is much larger than  $\Delta^{-1}$ . Therefore, assuming the existence of a mass gap, we expect that all the local quantities in  $G$  theory on  $T^4$  in the large volume limit should coincide with those in  $\tilde{G}$  theory on  $\mathbb{R}^4$ .

The spontaneous CP violation in  $\tilde{G}$  theory on  $\mathbb{R}^4$  can be probed by the expectation value  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{\tilde{G}}$ . In the following, instead, we investigate the  $\theta$ -dependence of  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,V}$  in  $G$  theory on  $T^4$ . In the presence of a mass gap, the finite volume correction is exponentially suppressed [22, 23]:

$$\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,V} - \langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,\infty} = O\left(\exp(-\Delta V^{1/4})\right). \quad (3.1)$$

This can be understood as follows. A theory on  $T^4$  is regarded as the same theory on  $\mathbb{R}^4$  with mirror images. The finite volume correction then comes from interactions with the mirror images which are suppressed exponentially as (3.1) since the distance to the nearest image is of order  $V^{1/4}$ . Since the difference between  $G$  theory and  $\tilde{G}$  theory comes from the global structure discussed in section 2, the quantity  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,\infty}$  should coincide with  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{\tilde{G}}$ . Therefore, if a phase transition would exist in  $G$  theory, then this implies the existence of the same phase transition in  $\tilde{G}$  theory which results in the spontaneous CP violation.

#### 3.1 The partition function

Recall that the partition function  $Z_G(\theta, V)$  of  $G$  theory is a periodic function of  $\theta$  with period  $2N\pi$  when  $V$  is finite. One might naively expect that the period of  $Z_G(\theta, V)$  would

become  $2\pi$  in the large volume limit since the effect of the twisted bundles would become irrelevant in the limit.

To clarify this issue, let us consider  $Z_G(\theta, V)$  in more detail. The relation (2.15) implies

$$\sum_{\nu} e^{i\theta(\nu - k_i m_i / N)} Z_G(k, m, \nu, V) = \sum_e e^{2\pi i k_i e_i / N} e^{-V F_G(e, m, \theta, V)}. \quad (3.2)$$

Using this relation and eq. (2.12),  $Z_G(\theta, V)$  can be written as

$$Z_G(\theta, V) = N^3 \sum_m e^{-V F_G(0, m, \theta, V)}, \quad (3.3)$$

where the summations over  $k$  and  $e$  have been performed.

We are interested in the values  $Z_G(2l\pi, V)$  with  $l = 0, 1, \dots, N-1$ . The relation (2.15) implies

$$F_G(e, m, \theta + 2l\pi, V) = F_G(e + lm, m, \theta, V), \quad (3.4)$$

which is nothing but the Witten effect [24]. This relation then implies

$$Z_G(2l\pi, V) = N^3 \sum_m e^{-V F_G(lm, m, 0, V)}. \quad (3.5)$$

Note that the fluxes appearing in the sum correspond to the line operators which are allowed to exist in the theories [6, 25, 26]. This is also the case for the partition function of  $\tilde{G}$  theory in eq. (2.13):

$$Z_{\tilde{G}}(\theta, V) = \sum_e e^{-V F_G(e, 0, \theta, V)}. \quad (3.6)$$

In the case  $l = 0$ , the fluxes in the sum are purely magnetic. In the confining phase, they are light, meaning that  $F_G(0, m, 0, V) - F_G(0, 0, 0, V)$  vanish exponentially in the large volume limit [17]. Therefore,  $Z_G(0, V)$  becomes

$$Z_G(0, V) \sim N^6 e^{-V F_G(0, 0, 0, V)} \quad (3.7)$$

for a large enough volume. On the other hand, the fluxes in the cases  $l \neq 0$  are heavy, i.e., the free energies do not vanish exponentially, except for  $m = 0$ . Since the contributions from the heavy fluxes are negligible, we obtain

$$Z_G(2\pi l, V) \sim N^3 e^{-V F_G(0, 0, 0, V)}. \quad (l = 1, 2, \dots, N-1) \quad (3.8)$$

This result clearly indicates that  $Z_G(\theta, V)$  has  $2N\pi$  periodicity even in the large volume limit. The ratio

$$Z_G(2\pi l, V) / Z_G(0, V) \sim N^{-3} \quad (3.9)$$

gives the ratio of the numbers of light fluxes.

The full partition function is also given by a Fourier series as follows:

$$Z_G(\theta, V) = \sum_P c_P(V) e^{iP\theta}, \quad P = 0, \pm \frac{1}{N}, \pm \frac{2}{N}, \dots \quad (3.10)$$

where the coefficients  $c_P(V)$  are given as

$$c_P(V) = \sum_{\nu + \frac{N-1}{N}k_i m_i = P} Z_G(k, m, \nu, V). \quad (3.11)$$

They are partition functions of the sector with a fixed  $P$  for  $\theta = 0$ , and thus they are real and positive (in the Euclidean theory). The existence of non-vanishing coefficients  $c_P(V)$  with fractional indices  $P$  is expected from the  $2N\pi$  periodicity of  $Z_G(\theta, V)$  even in the infinite volume limit, as long as the theory is in the confining phase at  $\theta = 0$ .

### 3.2 Mass gap

The results obtained so far can be applied to the free energy density, which we write as

$$F_G(\theta, V) := -\frac{1}{V} \log Z_G(\theta, V) = F_G(\theta, \infty) + g(\theta, V), \quad (3.12)$$

where  $g(\theta, V)$  represents the finite size correction. It was found that  $F_G(\theta, V)$  is  $2N\pi$  periodic, while  $F_G(\theta, \infty)$  should be  $2\pi$  periodic as it should coincide with the free energy in  $\tilde{G}$  theory up to a constant. Therefore, the finite size correction  $g(\theta, V)$  has  $2N\pi$  periodicity. Quantitatively, we found in the previous subsection that

$$g(2\pi, V) - g(0, V) \sim \frac{\log N^3}{V} \quad (3.13)$$

holds for a large enough volume.

The  $\theta$ -derivative of  $F_G(\theta, V)$  gives us the expectation value

$$\frac{1}{16\pi^2} \langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,V} = -\frac{i}{V} \frac{\partial}{\partial \theta} \log Z_G(\theta, V) = i \frac{\partial}{\partial \theta} F_G(\theta, \infty) + i \frac{\partial}{\partial \theta} g(\theta, V). \quad (3.14)$$

Since this is an expectation value of a local operator, its finite size correction  $i\partial_\theta g(\theta, V)$  should depend on the volume as  $\exp(-\Delta V^{1/4})$  [22, 23] in the presence of a mass gap  $\Delta$ . (See eq. (3.1).) Therefore, the derivative  $\partial_\theta g(\theta, V)$  should be exponentially suppressed at large  $V$ , implying that  $g(\theta, V)$  should be almost a constant in  $\theta$ .

The above arguments have the following consequence. Since  $g(\theta, V)$  is an almost constant function satisfying (3.13), a natural expectation for the functional form would be

$$g(\theta, V) \sim \begin{cases} g(0, V), & (0 \leq \theta \lesssim \theta_c) \\ g(0, V) + \frac{\log N^3}{V}, & (\theta_c \lesssim \theta \leq 2\pi) \end{cases} \quad (3.15)$$

for large enough  $V$ . By symmetry, we expect  $\theta_c = \pi$ . If this is indeed the case, then this indicates that the free energy density  $F_G(\theta, V)$  increases abruptly around  $\theta = \pi$ , indicating that the finite size correction  $i\partial_\theta g(\theta, V)$  becomes much larger than expected from the one due to the mass gap.



### 3.3 Phase transition

The appearance of a large finite size effect is a typical signature of a phase transition as we discuss below. In general, when we have a first-order phase transition, the partition function near the critical point  $\theta_c$  has the following form:

$$Z(\theta) \sim a_1 e^{-V f_1(\theta)} + a_2 e^{-V f_2(\theta)}, \quad (3.16)$$

where  $a_{1,2}$  are some coefficients of  $O(1)$  and  $f_{1,2}$  are free energy densities of two phases which satisfy

$$f_1(\theta_c) = f_2(\theta_c), \quad f'_1(\theta_c) \neq f'_2(\theta_c). \quad (3.17)$$

Here, the critical point  $\theta_c$  is defined as the one in the large  $V$  limit, and possible  $\theta$  and  $V$  dependencies of  $a_{1,2}$  can be ignored in the following discussion at a large enough volume.

Let us consider the log-derivative:

$$F'(\theta) := -\frac{1}{V} \frac{\partial}{\partial \theta} \log Z(\theta) \sim \frac{a_1 f'_1(\theta) e^{-V f_1(\theta)} + a_2 f'_2(\theta) e^{-V f_2(\theta)}}{a_1 e^{-V f_1(\theta)} + a_2 e^{-V f_2(\theta)}}, \quad (3.18)$$

which corresponds to the expectation value  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,V}$ . For large  $V$ ,  $F'(\theta)$  is equal to  $f'_1(\theta)$  or  $f'_2(\theta)$  up to exponentially suppressed terms if  $\theta$  is away from  $\theta_c$ . For  $\theta \sim \theta_c$ , on the other hand,  $F'(\theta)$  is approximately given by

$$F'(\theta) \sim \frac{a_1 f'_1(\theta) e^{-V f_1(\theta_c)(\theta - \theta_c)} + a_2 f'_2(\theta) e^{-V f_2(\theta_c)(\theta - \theta_c)}}{a_1 e^{-V f_1(\theta_c)(\theta - \theta_c)} + a_2 e^{-V f_2(\theta_c)(\theta - \theta_c)}}. \quad (3.19)$$

One can see that, in a region where  $|\theta - \theta_c| < O(1/V)$  in the unit of a typical energy scale  $\Delta$ , the value of  $F'(\theta)$  can deviate by  $O(1)$  from both  $f'_1(\theta)$  and  $f'_2(\theta)$ .

Applying this argument to the partition function  $Z_G(\theta, V)$ , it is concluded that  $\partial_\theta g(\theta, V)$  can become  $O(1)$  quantity in the region  $|\theta - \pi| < O(1/V)$ . Then, integration of  $\partial_\theta g(\theta, V)$  reproduces the expected functional form of  $g(\theta, V)$  in eq. (3.15). This strongly suggests that a first order phase transition exists at  $\theta = \pi$  in  $G$  theory.

In the infinite volume limit, the region where  $g(\theta, V)$  can vary disappears, and  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,V}$  develops a discontinuity at  $\theta = \pi$  due to the condition (3.17). Since  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,\infty}$  coincides with  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{\tilde{G}}$ , we conclude that the spontaneous CP violation occurs in  $\tilde{G}$  theory on  $\mathbb{R}^4$  at  $\theta = \pi$  since  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{\tilde{G}}$  is discontinuous there, as in the example of the softly broken  $\mathcal{N} = 1$  super Yang-Mills theory as well as large  $N$  theory. Remember that  $g(\theta, V)$  is a finite volume effect which disappears in the large volume limit. Nevertheless, it is interesting to note that its  $\theta$  and  $V$  dependencies tell us that a quantity on  $\mathbb{R}^4$ ,  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{\tilde{G}}$ , need to have a certain property; compatibility between the periodicity of the partition function encoded in  $g(\theta, V)$  and the mass gap requires a discontinuity in  $F'(\theta, \infty)$ .

The conclusion we obtained is consistent with the discussion based on the anomaly matching [8], there the cases of even and odd  $N$  are separately discussed. See also ref. [15] for detailed discussion on the case with odd  $N$ . Our discussion confirms that the same conclusion, spontaneous CP violation at  $\theta = \pi$ , can be derived independent of  $N$  under the assumptions that the mass gap persists for all values of  $\theta$  and a phase transition happens only once between  $\theta = 0$  and  $\theta = 2\pi$ .

We stress that the change (3.13) of  $g(\theta, V)$  as we vary  $\theta$  is a physical observable. First of all, *it can be measured by a lattice simulation*. This will be discussed in the next section. In addition, it has the following physical meaning. Recall that  $N^3$  is the number of light fluxes at  $\theta = 0$ . In the large volume limit, the light fluxes have almost zero energy, so  $N^3$  can be regarded as the partition function of a statistical system of the light fluxes. Therefore, the change in  $g(\theta, V)$  corresponds to the change in the entropy of these fluxes.

### 3.4 Other possibilities

So far, we have assumed the existence of a mass gap for any value of  $\theta$ . There is also a possibility, mainly for  $\tilde{G} = \text{SU}(2)$ , that the mass gap disappears, i.e., the deconfinement transition happens, at some point  $\theta = \theta_c$  or in some region.

Suppose that  $\Delta$  varies with  $\theta$  as

$$\Delta = O(|\theta - \theta_c|^a), \quad a > 0, \tag{3.20}$$

in the vicinity of the critical point  $\theta = \theta_c$ . As usual, we expect that the finite size effect would be relevant when  $1/\Delta > V^{1/4}$  is satisfied. Then, the range of  $\theta$  in which the finite size effect can become large is

$$|\theta - \theta_c| < O(V^{-1/4a}). \tag{3.21}$$

As was found in subsection 3.2,  $g(\theta, V)$  must change by the amount  $O(1/V)$  within this range. Then, the estimate of  $\partial_\theta g(\theta, V)$  around  $\theta = \theta_c$  is  $O(V^{1/(4a)-1})$ . In the case  $a > 1/4$ , the contribution from  $g(\theta, V)$  to  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{G,V}$  becomes negligible in the large  $V$  limit. Therefore,  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_G$  can be continuous in  $\theta$ , even though  $g(\theta, V)$  jumps at  $\theta = \theta_c$ . That is, it would be possible that the deconfinement transition happens at  $\theta = \pi$  without spontaneous CP violation.

If  $\Delta$  vanishes in a finite range of  $\theta$ , the phase transition happens twice at  $\theta = \theta_c$ , ( $0 < \theta_c < \pi$ ), and  $\theta = 2\pi - \theta_c$ . In this case, our argument so far cannot apply in the range  $\theta_c < \theta < 2\pi - \theta_c$ , and, for example,  $\langle F_{\mu\nu} \tilde{F}_{\mu\nu} \rangle_{\tilde{G}} = 0$  at  $\theta = \pi$  would be possible.

In summary, for consistency between the estimate of the finite size corrections and the confinement at  $\theta = 0$ , one either needs a first order phase transition or the disappearance of a mass gap at some value of  $\theta_c$ ,  $0 < \theta_c \leq \pi$ . In the case of the first order phase transition at  $\theta_c = \pi$ , there is spontaneous CP violation at  $\theta = \pi$ . In other cases, the CP invariant vacuum at  $\theta = \pi$  is possible.

## 4 Lattice study of $\text{SU}(N)/\mathbb{Z}_N$ theories

There have been efforts to investigate large  $\theta$  behavior of  $\text{SU}(N)$  theories at zero and finite temperatures on the lattice [27–29]. However, directly studying the  $\theta = \pi$  point is practically quite difficult due to the sign problem. The complex phase,  $e^{i\theta P}$ , prevents us from interpreting the integrand of the path integral as probabilities in Monte Carlo simulations. Instead, one can perform the path integral at  $\theta = 0$  and take the summation over the instanton numbers later with the phase factor as a weight to obtain a path integral

at non-zero  $\theta$  as in eq. (3.10). But, at  $\theta = \pi$ , the sum involves a numerical cancellation of order  $e^{-V\Delta^4\pi^2}$ , which makes it numerically and statistically not possible to obtain a meaningful result. The currently available techniques to simulate finite  $\theta$  are based on analytic continuation from imaginary values of  $\theta$  [28–31] or the reweighting method we just mentioned [27, 29]. Both methods work in a limited region close to  $\theta = 0$ .

We propose below a lattice study of the  $\theta$  dependence of  $G$  theory rather than  $\tilde{G}$  theory. Although the sign problem is as severe as  $\tilde{G}$  theory, the knowledge obtained in the previous section makes characteristic predictions on the distribution of indices  $P$  at  $\theta = 0$ . Using the knowledge as inputs, one should be able to improve the statistical uncertainties compared to the study of  $\tilde{G}$  theory. Also, by measuring the  $P$  distributions, one should be able to exclude the possibility of the phase transition significantly below  $\theta = \pi$  and also the case of the disappearing mass gap with a very small critical exponent.

On the lattice,  $\tilde{G}$  and  $G$  theories are formulated differently; the link variables are constructed as the fundamental and the adjoint representations of  $\tilde{G}$ , respectively [32, 33]. The partition function of the  $G$  theory is expressed as a path integral over the link variable in the adjoint representation,  $U_A$ , as

$$Z_G(\theta, \beta) = \int \mathcal{D}U_A e^{-\beta S[U_A] + i\theta P[U_A]}, \tag{4.1}$$

where

$$S[U_A] = \sum_{\text{plaquette}} \left( 1 - \frac{1}{N^2 - 1} \text{Tr} U_A^P \right), \tag{4.2}$$

and  $P[U_A]$  is the Pontryagin index calculated based on  $U_A$  which we discuss later. The matrix  $U_A^P$  is the plaquette action made of  $U_A$ . The partition function,  $Z_G(\theta, V)$ , is obtained by taking the continuum limit,  $\beta \rightarrow \infty$ , while the space-time volume,  $V$ , fixed.

In the actual simulation, one can use the link variable in the fundamental representation by using a relation between the characters in the adjoint and the fundamental representation; the trace of a group element,  $g$ , in the adjoint representation,  $\text{Tr} D_A(g)$ , can be expressed as  $|\text{Tr} D_F(g)|^2 - 1$  where  $D_F(g)$  is the same element in the fundamental representation [32, 33]. From this relation, the action of the  $G$  theory is given by the link variable  $U_F$  in the fundamental representation as

$$S[U_A] = \sum_{\text{plaquette}} \left( \frac{N^2}{N^2 - 1} - \frac{1}{N^2 - 1} |\text{Tr} U_F^P|^2 \right), \tag{4.3}$$

where  $U_F^P$  is the plaquette action made of  $U_F$ . The path integral measures are the same for the adjoint and the fundamental representations. In this formulation, we do not expect an increase of the computational cost compared to the  $\tilde{G}$  theory since the size of the matrix to be integrated remains the same.

As we discussed above, simulations with a large finite  $\theta$  are not practically easy. Instead, by the simulation at  $\theta = 0$ , one can measure the partition function of each  $P$  sector,  $c_P(V)$  in (3.10), as the probability of obtaining configurations with the index  $P$ . The index

can be measured in each configurations by counting zero modes of the Dirac operator in the adjoint representation through the index theorem,

$$P = \frac{n_+ - n_-}{2N}, \quad (4.4)$$

where  $n_{\pm}$  are the number of zero modes with  $\pm$  chiralities, and they should be even numbers as each mode is accompanied by its charge conjugate pair. The definition provides us with the index with the unit  $1/N$ . On the lattice, the Dirac operator which maintains the index theorem has been explicitly constructed [34], and by using the definition, the appearance of the configurations with fractional indices has been confirmed in  $SU(2)$  theory when the lattice spacing is finite [35], while it disappears in the continuum limit as expected [36]. As we discussed before, such configurations should remain unsuppressed even in the continuum limit in the  $SU(2)/\mathbb{Z}_2 \simeq SO(3)$  theory in the confining phase.

The distribution of  $P$ ,  $c_P(V)$ , has information of phase structures and the  $\theta$  dependence of  $G$  and  $\tilde{G}$  theories. It is expected that the configurations with fractional  $P$ 's frequently appear in the confining phase, but do not show up in the deconfining phase. Therefore, by heating up the system, by controlling the length of the temporal direction, we expect to see the suppression of the fractional  $P$  configurations at the deconfining temperature.

In the confining phase, interesting numbers to calculate are

$$\frac{Z_G(2l\pi, V)}{Z_G(0, V)} = \frac{\sum_P c_P(V) e^{2\pi i l P}}{\sum_P c_P(V)}, \quad l = 1, \dots, N-1, \quad (4.5)$$

which are given by  $1/N^3$  for all  $l$  in the large volume limit. The finite size correction to  $1/N^3$  is suppressed exponentially. This prediction does not depend on the detail of the phase structure along the  $\theta$  direction as long as the theory is in the confining phase at  $\theta = 0$ . It is an interesting observable which characterizes the confinement.

Let us discuss the  $P$  distribution at  $\theta = 0$ ,  $c_P(V)$ , in more detail. As we discussed in the previous section, the partition functions of the  $G$  and  $\tilde{G}$  theories at a sufficiently large volume are related by

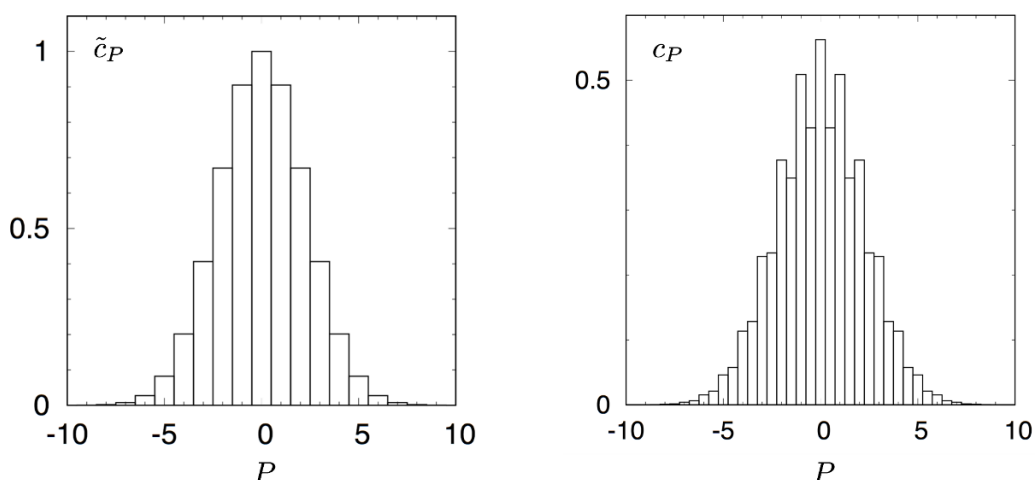
$$Z_G(\theta, V) \sim \begin{cases} N^6 Z_{\tilde{G}}(\theta, V), & |\theta| \lesssim \pi, \\ N^3 Z_{\tilde{G}}(\theta, V), & \pi \lesssim |\theta| \leq N\pi. \end{cases} \quad (4.6)$$

where

$$Z_{\tilde{G}}(\theta, V) = \sum_P \tilde{c}_P(V) e^{i\theta P}, \quad P = 0, \pm 1, \pm 2, \dots \quad (4.7)$$

From this relation, one can express  $c_P(V)$  in terms of  $\tilde{c}_P(V)$  as follows:

$$c_P(V) \propto \begin{cases} \frac{1}{N} \left( 1 + \frac{1}{N^2} - \frac{1}{N^3} \right) \tilde{c}_P(V), & P : \text{integer}, \\ \frac{1}{N} \left( 1 - \frac{1}{N^3} \right) \sum_{P'} \tilde{c}_{P'}(V) \frac{\sin[\pi(P - P')]}{\pi(P - P')}, & P : \text{non-integer}. \end{cases} \quad (4.8)$$



**Figure 1.** An example of the relation between  $\tilde{c}_P$  (left) and  $c_P$  (right) for  $N = 2$ .

The overall normalization is not important. By using this formula, once we measure  $c_P(V)$  with integer valued  $P$ , one can predict  $c_P(V)$  for non-integer  $P$ . The prediction is again not very sensitive to the behavior of  $Z_G(\theta, V)$  around  $\theta = \pi$  since the value there is anyway suppressed exponentially by the volume. A significant deviation from the above prediction means that  $Z_G(\theta, V)$  is deviated from eq. (4.6) in a wide range of  $\theta$ , that indicates either a phase transition at a small value of  $\theta$  or a very small critical exponent. We show in figure 1 the distribution predicted in eq. (4.8) for  $N = 2$  by assuming that  $\tilde{c}_P(V)$  is gaussian. We see an interesting non-smooth structure for small  $|P|$ .

Since there are  $N$  times more data points compared to  $\tilde{c}_P(V)$ , working in  $G$  theory should be advantageous in studying the  $P$  distribution, i.e., the  $\theta$  dependence of the theory. For example, when we parameterize the free energy in  $\tilde{G}$  theory as

$$F_{\tilde{G}}(\theta, V \rightarrow \infty) = \frac{\chi_t}{2} \theta^2 (1 + b_2 \theta^2 + b_4 \theta^4 + \dots), \tag{4.9}$$

the parameters,  $\chi_t, b_2, b_4, \dots$  can be determined by fitting the  $c_P(V)$  distribution. Compared to fitting with the  $\tilde{c}_P(V)$  distribution, one can use the constraints in eq. (4.8), which should help us to reduce the statistical uncertainties.

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