

Numerical studies on the finite-temperature CP restoration in 4D SU(N) gauge theory at $\theta = \pi$

Akira Matsumoto,^{a,*} Kohta Hatakeyama,^b Mitsuaki Hirasawa,^c Masazumi Honda,^{a,d} Jun Nishimura^{b,e} and Atis Yosprakob^f

^aRIKEN iTHEMS,

2-1 Hirosawa, Wako, Saitama 351-0198, Japan

^bKEK Theory Center, High Energy Accelerator Research Organization,

1-1 Oho, Tsukuba, Ibaraki 305-0801, Japan

^cSezione di Milano Bicocca, Istituto Nazionale di Fisica Nucleare,

Piazza della Scienza, 3, I-20126 Milano, Italy

^dCenter for Gravitational Physics and Quantum Information, Yukawa Institute for Theoretical Physics, Kyoto University, Sakyo-ku, Kyoto 606-8502, Japan

^eThe Graduate University for Advanced Studies, SOKENDAI,

1-1 Oho, Tsukuba, Ibaraki 305-0801, Japan

^fDepartment of Physics, Niigata University, Niigata 950-2181, Japan.

E-mail: akira.matsumoto@riken.jp, khat@post.kek.jp,

mitsuaki.hirasawa@mib.infn.it, masazumi318@gmail.com, jnishi@post.kek.jp,

ayosp@phys.sc.niigata-u.ac.jp

Recent studies on the 't Hooft anomaly matching condition have suggested a nontrivial phase structure in 4D SU(N) gauge theory at $\theta = \pi$. In the large- N limit, it has been found that CP symmetry at $\theta = \pi$ is broken in the confined phase, while it restores in the deconfined phase, which is indeed one of the possible scenarios. However, at small N , one may find other situations that are consistent with the consequence of the anomaly matching condition. Here we investigate this issue for $N = 2$ by direct lattice calculations. The crucial point to note is that the CP restoration can be probed by the sudden change of the tail of the topological charge distribution at $\theta = 0$, which can be seen by simulating the theory at imaginary θ without the sign problem. Our results suggest that the CP restoration at $\theta = \pi$ occurs at temperature higher than the deconfining temperature unlike the situation in the large- N limit.

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*Speaker

1. Introduction

The non-perturbative effect of the topological theta term in quantum field theories has been studied as a long-standing problem. Recently, the phase structure of 4D pure Yang-Mills (YM) theory with a theta term has attracted a lot of attention. There was a novel progress on application of 't Hooft anomaly matching [1, 2], which suggests that the 4D SU(N) pure YM theory cannot have a unique trivial vacuum at $\theta = \pi$. Indeed, this statement is consistent with the known phase diagram for large N , where the CP symmetry at $\theta = \pi$ is spontaneously broken in the confined phase. On the other hand, the phase diagram for small N , in particular $N = 2$, is not determined yet. It is possible that the SU(2) YM theory has a qualitatively different phase structure.

Thus, it is an interesting challenge to investigate the phase structure by a first-principle method. Since the effect of the theta term is genuinely non-perturbative, the SU(N) YM theory with a theta term should be analyzed by non-perturbative methods. However, usual Monte Carlo simulations of the lattice gauge theory including the theta term is difficult due to the sign problem.

We propose a new method to probe the critical behavior at $\theta = \pi$ based on the topological charge distribution $\rho(q)$ at $\theta = 0$. The crucial point of the method is that the expectation value $\langle Q \rangle_\theta$ of topological charge for any θ is completely determined by the distribution $\rho(q)$. Thanks to this property, we can investigate the behavior of $\langle Q \rangle_\theta$ indirectly by the information at $\theta = 0$. In order to see the temperature dependence of the distribution $\rho(q)$ clearly, we introduce the imaginary θ parameter, which can enhance the tail structure of $\rho(q)$.

2. Identifying the CP restoration

The application of 't Hooft anomaly matching condition [1, 2] to the 4D pure YM theory suggests that the phase structure at $\theta = \pi$ should be nontrivial. There are a lot of possible phase structures which agree with this condition. Here we consider two kinds of phase transition. One is the deconfinement transition at $T = T_{\text{dec}}(\theta = \pi)$, which corresponds to breaking of Z_N center symmetry. Note that the deconfining temperature $T_{\text{dec}}(\theta)$ depends on θ in general. The other transition is the restoration of CP symmetry at $T = T_{\text{CP}}$, which is broken at low temperature. For large N , these two transitions occur at the same temperature $T_{\text{CP}} = T_{\text{dec}}(\pi)$. Namely, the CP symmetry is recovered simultaneously with the deconfinement transition. In this case, either the Z_N center symmetry or the CP symmetry is broken at any temperature. Thus, it is consistent with the anomaly matching condition.

It is interesting to explore whether the theory with $N = 2$ has a similar phase diagram. In fact, the numerical study of 4D SU(2) YM theory by the subvolume method [3, 4] shows an indication of the CP broken phase at low temperature. It is also confirmed that the instanton gas phase, which is CP symmetric, appears at high temperature. Thus, the restoration of CP symmetry is expected to occur also for $N = 2$. However, the relation between the two critical temperatures T_{CP} and $T_{\text{dec}}(\pi)$ can be different. The anomaly matching condition for these two temperatures requires that $T_{\text{CP}} \geq T_{\text{dec}}(\pi)$. The reason is that the CP symmetry can be broken not only in the confined phase but also in the deconfined phase. The overlap of the CP broken phase and the Z_2 broken phase is allowed. There is a related study of these two critical temperatures by using the super YM theory [5]. Interestingly, the result shows $T_{\text{CP}} > T_{\text{dec}}(\pi)$ only for $N = 2$, but $T_{\text{CP}} = T_{\text{dec}}(\pi)$ for $N \geq 3$.

It is worth trying to numerically investigate the CP restoration temperature T_{CP} for the 4D SU(2) YM theory and compare it with the deconfining temperature $T_{\text{dec}}(\pi)$. However, the usual Monte Carlo simulation at $\theta = \pi$ suffers from the sign problem since the theta term is purely imaginary. In this section we introduce a new method to determine T_{CP} without direct simulation at $\theta = \pi$.

First, we explain the property of topological charge Q . Since the topological charge is a CP odd operator, its expectation value $\langle Q \rangle_\theta$ can be an order parameter of CP symmetry.

$$\langle Q \rangle_\theta = -i \frac{\partial}{\partial \theta} \log Z_\theta \quad (1)$$

If CP symmetry at $\theta = \pi$ is spontaneously broken, $\langle Q \rangle_\theta$ should be discontinuous there:

$$\Delta Q = \left| \langle Q \rangle_{\theta=\pi-\epsilon} - \langle Q \rangle_{\theta=\pi+\epsilon} \right| \begin{cases} > 0 & : \text{CP broken,} \\ = 0 & : \text{CP restored.} \end{cases} \quad (2)$$

Thus, the CP restoration temperature T_{CP} can be regarded as a temperature at which ΔQ vanishes. To determine T_{CP} , we need to investigate the temperature dependence of ΔQ . However, it is difficult to directly evaluate ΔQ due to the sign problem. But we can also study it from another direction. Let us note that the partition function Z_θ and the topological charge distribution $\rho(q)$ at $\theta = 0$ are related via

$$\rho(q) = \frac{1}{Z_0} \int dA \delta(q - Q) e^{-S_g} = \frac{1}{Z_0} \int \frac{d\theta}{2\pi} e^{-i\theta q} Z_\theta. \quad (3)$$

Since the distribution $\rho(q)$ is a Fourier transform of the partition function Z_θ ,

$$Z_\theta = \int dA e^{-S_g + i\theta Q} = Z_0 \int dq e^{i\theta q} \rho(q), \quad (4)$$

we find that the expectation value $\langle Q \rangle_\theta$ at any θ is completely determined by $\rho(q)$ as

$$\langle Q \rangle_\theta = -i \frac{\partial}{\partial \theta} \log \int dq e^{i\theta q} \rho(q) = \frac{\int dq q e^{i\theta q} \rho(q)}{\int dq e^{i\theta q} \rho(q)}. \quad (5)$$

This is nothing but the reweighting formula by using the information at $\theta = 0$. Thus, to calculate $\langle Q \rangle_\theta$ around $\theta \sim \pi$, we need exponentially large amount of statistics. However, our goal is not to determine the complete θ dependence of $\langle Q \rangle_\theta$ but to probe the critical temperature T_{CP} . In fact, we do not need the complete information of $\rho(q)$ in that case. It is enough to determine whether ΔQ is zero or not from $\rho(q)$.

In this study, we propose to use the expectation value $\langle Q \rangle_{\tilde{\theta}}$ of the topological charge at an imaginary theta $\theta = i\tilde{\theta}$ ($\tilde{\theta} \in \mathbb{R}$) to probe the critical behavior;

$$\langle Q \rangle_{\tilde{\theta}} = \frac{1}{Z_{\tilde{\theta}}} \int dA Q e^{-S_g - \tilde{\theta} Q} = \frac{\int dq q e^{-\tilde{\theta} q} \rho(q)}{\int dq e^{-\tilde{\theta} q} \rho(q)}. \quad (6)$$

In practice, we normalize it by the topological susceptibility

$$\chi_0 = \frac{1}{V} \langle Q^2 \rangle_{\theta=0} \quad (7)$$

at $\theta = 0$ and the volume V , so that we just measure the ratio of two independent observables.

$$\frac{\langle Q \rangle_{\tilde{\theta}}}{\chi_0 V} = \frac{\langle Q \rangle_{\tilde{\theta}}}{\langle Q^2 \rangle_0} \quad (8)$$

Let us discuss the behavior of this observable in some well known models. The first example is the instanton gas model, for which the free energy is obtained as

$$F_\theta = -\log Z_\theta = \chi_0 V (1 - \cos \theta). \quad (9)$$

The θ -dependence of $\langle Q \rangle_\theta / \chi_0 V$ for real θ is given by the sine function

$$\frac{\langle Q \rangle_\theta}{\chi_0 V} = i \sin \theta, \quad (10)$$

which indicates that CP symmetry at $\theta = \pi$ is not broken. Correspondingly, the imaginary- θ dependence turns out to be the hyperbolic sine function.

$$\frac{\langle Q \rangle_{\tilde{\theta}}}{\chi_0 V} = -\sinh \tilde{\theta} \quad (11)$$

The second example is the Gaussian model

$$F_\theta = \frac{1}{2} \chi_0 V \min_n (\theta - 2\pi n)^2, \quad (12)$$

which is known to be realized for large N at low temperature. The real- θ dependence of $\langle Q \rangle_\theta / \chi_0 V$ is given by

$$\frac{\langle Q \rangle_\theta}{\chi_0 V} = i(\theta \bmod 2\pi) \quad (13)$$

for $V \gg 1$, which indicates that the CP is broken. For imaginary θ , we find the linear behavior.

$$\frac{\langle Q \rangle_{\tilde{\theta}}}{\chi_0 V} = -\tilde{\theta} \quad (14)$$

We can see the clear difference between the behaviors of $\langle Q \rangle_{\tilde{\theta}} / \chi_0 V$ for these two models. It behaves as $-\sinh \tilde{\theta}$ for the instanton gas model (CP restored), while it behaves as $-\tilde{\theta}$ for the Gaussian model (CP broken). Although the 4D SU(2) YM theory will not be as simple as these models, this observable is still useful to investigate the CP restoration. In fact, the expectation value $\langle Q \rangle_{\tilde{\theta}}$ for imaginary θ is sensitive to the tail of the distribution of $\rho(q)$. The imaginary theta term enhances the contribution of large- q sectors because of the factor $e^{-\tilde{\theta}q}$ in the integrand of (6). Note that, for these two examples, the tail of $\rho(q)$ behaves for $q \gg 1$ as follows:

$$\rho(q) \sim \begin{cases} \exp\left(-q \log \frac{2q}{\chi_0 V}\right) & : \text{instanton gas,} \\ \exp\left(-\frac{q^2}{2\chi_0 V}\right) & : \text{Gaussian.} \end{cases} \quad (15)$$

3. 4D SU(2) gauge theory with a theta term

In this study, we focus on the SU(2) pure Yang-Mills theory on the 4D Euclidean space. The action for the gauge field A_μ^a ($a = 1, 2, 3$) ($\mu = 1, \dots, 4$) is defined by

$$S_g = \frac{1}{4g^2} \int d^4x F_{\mu\nu}^a F_{\mu\nu}^a, \quad (16)$$

where g is the coupling constant and $F_{\mu\nu}^a$ is the field strength.

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - \epsilon^{abc} A_\mu^b A_\nu^c \quad (17)$$

The topological charge is given by

$$Q = \frac{1}{64\pi^2} \int d^4x \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a F_{\rho\sigma}^a, \quad (18)$$

which takes an integer value on the compact space. We introduce the topological theta term $S_\theta = -i\theta Q$ with a parameter $\theta \in \mathbb{R}$, so that the total action is $S = S_g + S_\theta$. Since the partition function

$$Z = \int \mathcal{D}A e^{-S_g + i\theta Q} \quad (19)$$

is invariant under the shift $\theta \rightarrow \theta + 2\pi$, the theory has 2π periodicity with respect to θ . Since the parameter θ flips its sign by the CP transformation $\theta \rightarrow -\theta$, the theta term explicitly breaks the CP symmetry for $\theta \neq 0$. However, thanks to the 2π periodicity, the CP symmetry exists also at $\theta = \pi$.

Next, we define the lattice action for the numerical study. The gauge field is represented by the link variable $U_{n,\mu} \in \text{SU}(2)$. The index n labels the lattice sites. The plaquette is given by

$$P_n^{\mu\nu} = U_{n,\mu} U_{n+\hat{\mu},\nu} U_{n+\hat{\nu},\mu}^\dagger U_{n,\nu}^\dagger, \quad (20)$$

where $\hat{\mu}$ represents the unit vector along the μ -th direction. Then we define the plaquette action with the lattice coupling constant β .

$$S_g = -\frac{\beta}{4} \sum_n \sum_{\mu \neq \nu} \text{Tr}(P_n^{\mu\nu}) \quad (21)$$

Similarly, we can define the topological charge on the lattice by the so-called "clover leaf" formula, [6]

$$Q_{\text{cl}} = -\frac{1}{32\pi^2} \sum_n \frac{1}{2^4} \sum_{\mu,\nu,\rho,\sigma=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \text{Tr}(P_n^{\mu\nu} P_n^{\rho\sigma}). \quad (22)$$

Here the orientation of the plaquette is extended to the negative directions as well. The corresponding anti-symmetric tensor $\tilde{\epsilon}_{\mu\nu\rho\sigma}$ also has negative indices, so that

$$1 = \tilde{\epsilon}_{1234} = -\tilde{\epsilon}_{2134} = -\tilde{\epsilon}_{-1234} = \dots \quad (23)$$

It is known that the naively defined topological charge Q_{cl} does not take an integer value on the lattice due to the discretization effect. In order to recover the topological property of the gauge field, we need to eliminate short-range fluctuations. In fact, there are some smoothing techniques, such as the gradient flow, stout smearing and so on. By using such a technique, we can define the smeared topological charge so that it becomes close to an integer. In this study, we introduce the stout smearing to the hybrid Monte Carlo simulation, which is discussed in section 4.

4. Stout smearing for the HMC

Since the CP symmetry at $\theta = \pi$ is related to the 2π periodicity of θ , the topological property of the theory is essential in the study of the phase structure. Thus, we use the stout smearing [7] to define the topological charge. In the hybrid Monte Carlo simulation, the drift force is used to update the configuration. If the action has the theta term with the smeared topological charge, it also contributes to the drift force. We can explicitly calculate the drift force from the smeared topological charge by using stout smearing. In this section, we briefly review the stout smearing in the hybrid Monte Carlo simulation.

Stout smearing is an iterative procedure to obtain the smeared link $\tilde{U}_{n,\mu}$ starting from the original link $U_{n,\mu}$. We call the number of iterations N_ρ .

$$U_{n,\mu} = U_{n,\mu}^{(0)} \rightarrow U_{n,\mu}^{(1)} \rightarrow \cdots \rightarrow U_{n,\mu}^{(N_\rho)} = \tilde{U}_{n,\mu}. \quad (24)$$

In one (isotropic) smearing step from k to $k+1$, the link variable $U_{n,\mu}^{(k)} \in \text{SU}(2)$ is mapped to $U_{n,\mu}^{(k+1)} \in \text{SU}(2)$ defined by following formulae:

$$U_{n,\mu}^{(k+1)} = e^{iY_{n,\mu}} U_{n,\mu}^{(k)}, \quad (25)$$

$$iY_{n,\mu} = -\frac{\rho}{2} \text{Tr}(J_{n,\mu} \tau^a) \tau^a, \quad (26)$$

$$J_{n,\mu} = U_{n,\mu} \Omega_{n,\mu} - \Omega_{n,\mu}^\dagger U_{n,\mu}^\dagger, \quad (27)$$

$$\Omega_{n,\mu} = \sum_{\sigma (\neq \mu)} \left(U_{n+\hat{\mu},\sigma} U_{n+\hat{\sigma},\mu}^\dagger U_{n,\sigma}^\dagger + U_{n+\hat{\mu}-\hat{\sigma},\sigma}^\dagger U_{n-\hat{\sigma},\mu}^\dagger U_{n-\hat{\sigma},\sigma} \right). \quad (28)$$

Here τ^a are the SU(2) generators in fundamental representation. The smearing step parameter $\rho > 0$ should be chosen appropriately depending on the system.

In the hybrid Monte Carlo simulation, we obtain the smeared link $\tilde{U}_{n,\mu}$ by this procedure, and then we use $\tilde{U}_{n,\mu}$ to calculate the topological charge (22) instead of the original link $U_{n,\mu}$. The topological charge given by the stout smearing

$$Q := Q_{\text{cl}}(\tilde{U}) \quad (29)$$

is used in the theta term $S_\theta = -i\theta Q$ as well as in measuring the observable. In the step of molecular dynamics, we need to calculate the drift force

$$F_{n,\mu} = i\tau^a D_{n,\mu}^a S_\theta \quad (30)$$

from the theta term. Although S_θ is a complicated function of the original link variable $U_{n,\mu}$, it is possible to calculate the drift force by reversing the smearing steps (24).

5. Result of the HMC

In this section, we show the result of the hybrid Monte Carlo simulation with the imaginary theta term. For the stout smearing, we set $N_\rho = 40$ and $\rho = 0.09$ so that the topological charge is close to an integer. In Fig. 1, we plot $-\langle Q \rangle_{\tilde{\theta}} / \chi_0 V$ against $\tilde{\theta}/\pi = \theta/i\pi$ for various values of temperature

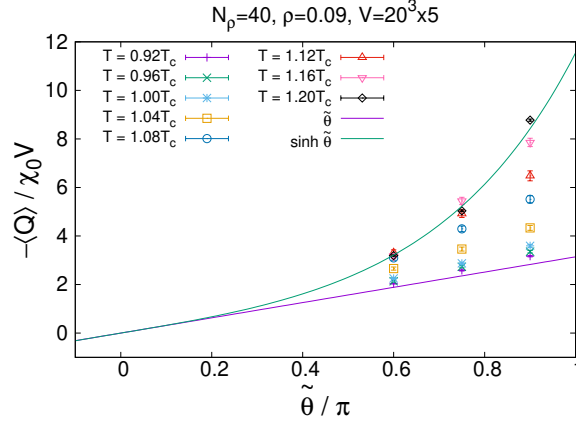


Figure 1: The imaginary θ dependence of $-\langle Q \rangle_{\tilde{\theta}} / \chi_0 V$ for various values of temperature in $0.92 \leq T/T_{\text{dec}}(0) \leq 1.20$ with increments of 0.04. The green solid curve is obtained by the instanton gas approximation, which is valid at high temperature. The purple solid line is obtained by the Gaussian model.

in the range $0.9 \leq T/T_{\text{dec}}(\theta = 0) \leq 1.2$. We found that, at high temperature, the data points are consistent with the instanton gas approximation. On the other hand, the data points approach the behavior of the Gaussian model at low temperature. It is convincing that the SU(2) YM theory behaves as the instanton gas model at high temperature. However, it does not necessarily coincide with the Gaussian model at low temperature since the situation of $N = 2$ can be different from that of large N . Nevertheless, this observable is suitable for probing the phase structure. Indeed, we can see that the behaviors of $\langle Q \rangle_{\tilde{\theta}} / \chi_0 V$ change drastically slightly above the deconfining temperature $T_{\text{dec}}(0)$ at $\theta = 0$.

In order to see the temperature dependence of $-\langle Q \rangle_{\tilde{\theta}} / \chi_0 V$, we plot it against temperature at fixed $\theta/\pi = 0.75i$ in Fig. 2. The left figure is the result for $V = 16^3 \times 5$, and the right figure is the result for $V = 20^3 \times 5$. The yellow curve shows the result of fitting by a cubic function $f(x) = ax^3 + bx^2 + cx + d$ where a, b, c and d are fitting parameters. The orange curve is the derivative of $f(x)$. We find that the derivative is the largest at around $T_{\text{peak}} \sim 1.06T_{\text{dec}}(0)$. We also find that the height of the peak grows as the spatial volume V_s increases.

In Fig. 3(left), we plot the peak position $T_{\text{peak}}/T_{\text{dec}}(0)$ against $1/V_s$ obtained by the same analysis for $\theta/\pi = 0.6i, 0.75i$ and $0.9i$. The significant volume dependence of T_{peak} is not observed. These results suggest that there is a phase transition around $T/T_{\text{dec}}(0) \sim 1.06$. In Fig. 3(right), the peak height of the fitting function is plotted against $V_s^{1/3}$. This non-linear finite size scaling suggests that the phase transition is of the second order or higher.

The existence of the transition indicates that the distribution $\rho(q)$ of the topological charge changes drastically around $T/T_{\text{dec}}(0) \sim 1.06$. Assuming that CP symmetry at $\theta = \pi$ is spontaneously broken at low temperature, the drastic change of $\rho(q)$ should correspond to the critical behavior of $\langle Q \rangle_{\theta=\pi}$. Thus, we identify the critical temperature T_{peak} as the CP restoration temperature T_{CP} , which suggests $T_{\text{CP}} > T_{\text{dec}}(0)$.

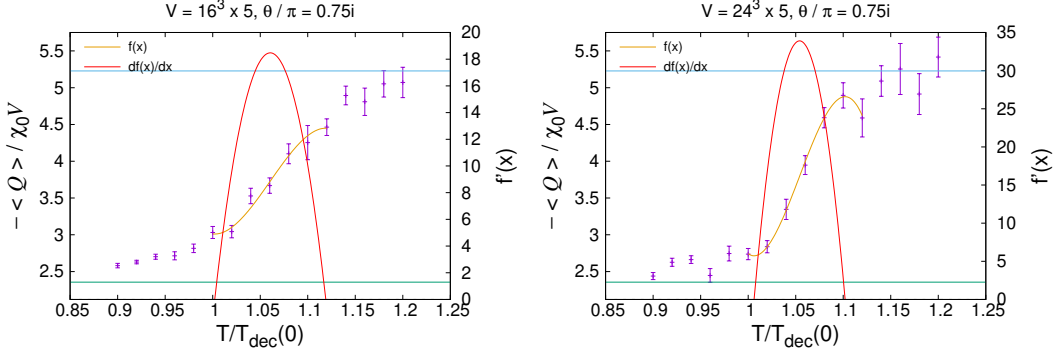


Figure 2: The temperature dependence of $-\langle Q \rangle_{\theta} / \chi_0 V$ at $\theta/\pi = 0.75i$ for $V = 16^3 \times 5$ (left) and $V = 20^3 \times 5$ (right). We fit the data points by a cubic function $f(x) = ax^3 + bx^2 + cx + d$. The orange solid line shows the result of fitting. The red solid line is derivative of $f(x)$ with respect to x .

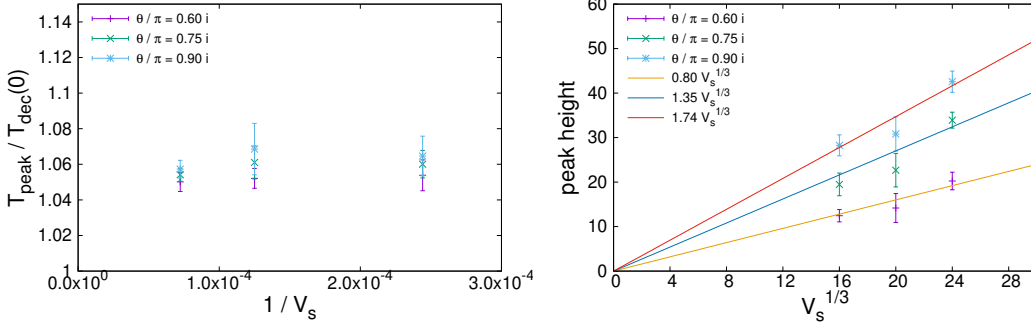


Figure 3: (left) The peak position $T_{\text{peak}}/T_{\text{dec}}(0)$ against $1/V_s$ for $\theta/\pi = 0.60i$, $0.75i$ and $0.90i$, where V_s is the spacial lattice volume. (right) The peak height of $f'(x)$ is plotted against $V_s^{1/3}$. The straight lines represent the fit to the behavior $aV_s^{1/3}$.

6. Summary

Recent studies on the 't Hooft anomaly matching condition for the 4D SU(N) gauge theory have suggested that the phase structure at $\theta = \pi$ should be nontrivial. For large N , it is known that the CP symmetry at $\theta = \pi$ is spontaneously broken in the confined phase, while it is restored in the deconfined phase. However, for small N , a qualitatively different phase structure can be realized, as long as the anomaly matching condition is satisfied. In this work, we investigated this issue for $N = 2$ by hybrid Monte Carlo simulation of lattice gauge theory. We probed the restoration of the CP symmetry by a sudden change of the topological charge distribution at $\theta = 0$, which can be seen by simulating the theory with imaginary θ . This method is free from the sign problem. We measured the normalized expectation value $\langle Q \rangle / \chi_0 V$ of the topological charge as a probe of the distribution. We found that this observable has a finite-temperature transition around $T/T_{\text{dec}}(0) \sim 1.06$.

Although the deconfinement temperature T_{dec} at $\theta = \pi$ is not known, it is expected to be lower than $T_{\text{dec}}(0)$. Thus, our results suggest that the CP symmetry at $\theta = \pi$ is restored at the temperature higher than the deconfinement temperature—unlike the situation at large N . We plan to refine this

result by taking the continuum limit. We are also trying to extend this method to the 4D SU(3) YM theory, in order to see a possible qualitative difference between $N = 2$ and $N = 3$, as suggested from the result in super YM theory.

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