

A new technique for solving the freezing problem in the complex Langevin simulation of 4D SU(2) gauge theory with a theta term

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We apply the complex Langevin method (CLM) to overcome the sign problem in 4D SU(2) gauge theory with a theta term extending our previous work on the 2D U(1) case. The topology freezing problem can be solved by using open boundary conditions in all spatial directions, and the criterion for justifying the CLM is satisfied even for large θ as far as the lattice spacing is sufficiently small. However, we find that the CP symmetry at $\theta = \pi$ remains to be broken explicitly even in the continuum and infinite-volume limits due to the chosen boundary conditions. In particular, this prevents us from investigating the interesting phase structures suggested by the 't Hooft anomaly matching condition. We also try the so-called subvolume method, which turns out to have a similar problem. We therefore discuss a new technique within the CLM, which enables us to circumvent the topology freezing problem without changing the boundary conditions.

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1. Introduction

We can explore the topological nature of quantum field theories via topological terms. Recently, gauge theories with a theta term have been studied by 't Hooft anomaly matching. In particular, there is a constraint on the phase structure of the 4D SU(N) pure Yang-Mills theory by a 't Hooft anomaly involving the CP and center symmetries at $\theta = \pi$ [1]. The constraint is consistent with the well-known scenario at large N [2], where the theory at $\theta = \pi$ is confined with spontaneously broken CP at low temperature and then has a transition to deconfined phase with restored CP at a finite temperature. However, it is highly nontrivial whether or not this structure persists for small N since there are various ways to satisfy the anomaly matching condition. For instance, the theory for small N at low temperature may be deconfined or gapless as well as spontaneously broken CP. Therefore it is an interesting challenge to investigate the phase structure by first-principle calculation at the smallest N i.e. $N = 2$. The effect of the theta term is genuinely non-perturbative. The theory with a theta term should be analyzed by non-perturbative calculations based on the lattice gauge theory. However, the Monte Carlo simulation of the theory including the theta term is difficult due to the sign problem.

The complex Langevin method (CLM) is one of the approaches which allow us to avoid the sign problem [3–8]. We use the CLM to study 4D SU(2) gauge theory with the theta term since its computational cost is cheaper than the other methods. The topological charge on the 4D lattice is contaminated by short range fluctuations. Thus, we apply the stout smearing [9] to recover the topological property. In this method, the effect of the smearing can be included dynamically. We discuss the behavior of the topological charge for $\theta \neq 0$ in the CLM.

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

We consider 4D SU(2) gauge theory on the Euclidean space. The action for the gauge field A_μ^a ($a = 1, 2, 3$) ($\mu = 1, \dots, 4$) is given by

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

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

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - \epsilon^{abc} A_\mu^b A_\nu^c. \quad (2)$$

The topological charge Q is defined by

$$Q = \frac{1}{64\pi^2} \int d^4x \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a F_{\rho\sigma}^a, \quad (3)$$

which takes integer values unless the space has a boundary. We introduce the theta term $S_\theta = -i\theta Q$, and thus the action is $S = S_g + S_\theta$. This theory has the 2π periodicity of the parameter $\theta \in \mathbb{R}$, since the partition function

$$Z = \int \mathcal{D}A e^{-S_g + i\theta Q} \quad (4)$$

is invariant under the shift $\theta \rightarrow \theta + 2\pi$.

Next, we consider the lattice action for the numerical study. We introduce link variables $U_{n,\mu} \in \text{SU}(2)$ and define plaquettes.

$$P_n^{\mu\nu} = U_{n,\mu} U_{n+\hat{\mu},\nu} U_{n+\hat{\nu},\mu}^{-1} U_{n,\nu}^{-1} \quad (5)$$

The index n labels the lattice site and $\hat{\mu}$ represents the unit vector along the μ -th direction. Note that we use $U_{n,\mu}^{-1}$ instead of $U_{n,\mu}^\dagger$ to respect holomorphicity, which is necessary to justify the CLM. We define the plaquette action by

$$S_\beta = -\frac{\beta}{4} \sum_n \sum_{\mu \neq \nu} \text{Tr} P_n^{\mu\nu} \quad (6)$$

with the coupling constant β . For the topological charge on the lattice, we consider the simplest discretization [10] given by the so called "clover leaf" formula.

$$Q_{\text{cl}} = -\frac{1}{32\pi^2} \sum_n \frac{1}{2^4} \sum_{\mu,\nu,\rho,\sigma=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \text{Tr} [P_n^{\mu\nu} P_n^{\rho\sigma}] \quad (7)$$

Here the orientation of the plaquette is generalize to negative directions. Correspondingly, the anti-symmetric tensor $\tilde{\epsilon}_{\mu\nu\rho\sigma}$ also has negative indices, for example

$$1 = \tilde{\epsilon}_{1234} = -\tilde{\epsilon}_{2134} = -\tilde{\epsilon}_{(-1)234} = \dots \quad (8)$$

Usually the topological charge Q_{cl} does not take integer values on the lattice due to the discretization effect. We can recover the topological property of the gauge field by eliminating short-range fluctuations. Some smoothing techniques, such as the gradient flow, stout smearing and so on, make the topological charge close to integers. In this study, we apply the stout smearing to the complex Langevin method, which is discussed in section 4.

3. Complex Langevin method

Since the theta term is purely imaginary, Monte Carlo studies of the theory with $\theta \neq 0$ is extremely difficult due to the sign problem. We avoid this problem by using the complex Langevin method (CLM) [3–8], which is a generalization of the Langevin method to the system with a complex action. Its computational cost grows linearly with the system size, so that we can easily apply the CLM to large systems in a straightforward manner. In this section, we briefly review how to apply the method to 4D SU(2) gauge theory.

In the CLM, we consider a fictitious time evolution of the dynamical variables, which is described by the complex Langevin equation. The discretized complex Langevin equation for the link variables is given by

$$U_{n,\mu}(t + \epsilon) = \exp \left[-i\epsilon D_{n,\mu}^a \mathcal{S} \tau^a + i\sqrt{\epsilon} \eta_{n,\mu}(t) \right] U_{n,\mu}(t), \quad (9)$$

where $\tau^a = \sigma^a/2$ are the generators of SU(2). The parameter $\epsilon \ll 1$ is a step size of the discretized fictitious time. The differential operation $D_{n,\mu}^a f$ of the function $f(U)$ with respect to the link variables (Lie group elements) is defined by

$$D_{n,\mu}^a f(U_{n,\mu}) = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[f \left(e^{i\epsilon \tau^a} U_{n,\mu} \right) - f(U_{n,\mu}) \right]. \quad (10)$$

The term including $D_{n,\mu}^a S$ is called the drift term. The other term is a real Gaussian noise $\eta_{n,\mu}(t) = \eta_{n,\mu}^a(t)\tau^a$ normalized by

$$\langle \eta_{n,\mu}^a(t)\eta_{m,\nu}^b(t') \rangle = 2\delta_{nm}\delta_{\mu\nu}\delta^{ab}\delta_{tt'}. \quad (11)$$

The drift term $D_{n,\mu}^a S$ is no longer Hermitian for the complex action. Thus, the link variables deviate from SU(2) in the complex Langevin simulation. We treat the link variables as SL(2, \mathbb{C}) elements instead of SU(2), which corresponds to complexifying the gauge field. For the complexified configuration, the drift term and observables should also be complexified respecting holomorphicity.

The expectation value of \mathcal{O} is calculated from an ensemble of configurations, which is given by solving the complex Langevin equation numerically. We can obtain the expectation value $\langle \mathcal{O} \rangle_{\text{CLM}}$ as an average of $\mathcal{O}(U)$ in the ensemble. However, it will not always agree with the correct expectation value defined by the path integral. This problem is known as the wrong convergence of the CLM, which occurs depending on the system, the parameter and the choice of the dynamical variables. Although we cannot figure out whether the problem occurs or not a priori, there is a practical criterion for the correct convergence [8]. We obtain the correct expectation value $\langle \mathcal{O} \rangle_{\text{CLM}} = \langle \mathcal{O} \rangle$ only if the probability distribution of the drift term falls off exponentially or faster. We can easily check the criterion by plotting the histogram of the magnitude u of the largest drift defined by

$$u = \frac{1}{\sqrt{2}} \max_{n,\mu} \|D_{n,\mu}^a S\tau^a\|, \quad (12)$$

where the norm of the matrix is defined by $\|A\|^2 := \text{Tr}[A^\dagger A]$.

We can stabilize the complex Langevin simulation by using a technique called "gauge cooling" [11]. The condition of the correct convergence tends to be violated if the link variables deviate far away from SU(2). The gauge cooling reduces the non-unitarity of link variables as much as possible. Thus, it helps the condition to be satisfied. It was also shown that this procedure does not affect any gauge invariant observable [7, 8]. We apply the gauge cooling at each Langevin step in order to suppress a rapid growth of non-unitarity.

4. Stout smearing for the CLM

The theory with a theta term has the 2π periodicity of θ , which plays an important role in the appearance of the nontrivial phase structure at $\theta = \pi$. However, it is difficult to retain this property on the lattice because the topological charge (7) defined by the naive discretization does not take integer values. It approaches integers only for the configurations sufficiently close to the continuum limit. In fact, it is difficult to suppress the short range fluctuations enough simply by increasing β . Thus, we need a smearing method which makes the configuration sufficiently smooth even for small β . In this work, we use the stout smearing [9], which is applicable to the CLM. In fact, its application to the CLM was discussed in the analysis of QCD at nonzero baryon density [12]. In this section, we review how to apply the stout smearing to the complex Langevin simulation of the gauge theory with the theta term.

The procedure of the stout smearing is given by the iteration of the smearing step, starting from the original configuration $U_{n,\mu}$.

$$U_{n,\mu} = U_{n,\mu}^{(0)} \rightarrow U_{n,\mu}^{(1)} \rightarrow \dots \rightarrow U_{n,\mu}^{(N_\rho)} = \tilde{U}_{n,\mu} \quad (13)$$

After N_ρ iterations we obtain the smeared configuration $\tilde{U}_{n,\mu}$. In one (isotropic) smearing step from k to $k+1$, the link variable $U_{n,\mu}^{(k)} \in \text{SL}(2, \mathbb{C})$ is mapped to $U_{n,\mu}^{(k+1)} \in \text{SL}(2, \mathbb{C})$ defined by following formulae.

$$U_{n,\mu}^{(k+1)} = e^{iY_{n,\mu}} U_{n,\mu}^{(k)} \quad (14)$$

$$iY_{n,\mu} = -\frac{\rho}{2} \text{Tr} [J_{n,\mu} \tau^a] \tau^a \quad (15)$$

$$J_{n,\mu} = U_{n,\mu} \Omega_{n,\mu} - \bar{\Omega}_{n,\mu} U_{n,\mu}^{-1} \quad (16)$$

$$\Omega_{n,\mu} = \sum_{\sigma(\neq\mu)} \left(U_{n+\hat{\mu},\sigma} U_{n+\hat{\sigma},\mu}^{-1} U_{n,\sigma}^{-1} + U_{n+\hat{\mu}-\hat{\sigma},\sigma}^{-1} U_{n-\hat{\sigma},\mu}^{-1} U_{n-\hat{\sigma},\sigma} \right) \quad (17)$$

$$\bar{\Omega}_{n,\mu} = \sum_{\sigma(\neq\mu)} \left(U_{n,\sigma} U_{n+\hat{\sigma},\mu} U_{n+\hat{\mu},\sigma}^{-1} + U_{n-\hat{\sigma},\sigma}^{-1} U_{n-\hat{\sigma},\mu} U_{n+\hat{\mu}-\hat{\sigma},\sigma} \right) \quad (18)$$

The parameter $\rho > 0$ should be chosen appropriately, depending on the system.

We use the topological charge (7) calculated from the smeared configuration $\tilde{U}_{n,\mu}$

$$Q := Q_{\text{cl}}(\tilde{U}) \quad (19)$$

to define the theta term $S_\theta = -i\theta Q$ on the lattice. For the complex Langevin simulation, we need to calculate the drift term $D_{n,\mu}^a S_\theta$ 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

$$F_{n,\mu} = i\tau^a D_{n,\mu}^a S_\theta \quad (20)$$

by reversing the smearing steps (13). We define the drift force for the link variables $U_{n,\mu}^{(k)}$ as

$$F_{n,\mu}^{(k)} = i\tau^a D_{n,\mu}^{(k)a} S_\theta, \quad (21)$$

where $D_{n,\mu}^{(k)a}$ represents a differential operation with respect to $U_{n,\mu}^{(k)}$. As a first step to calculate (20), the calculation of the drift force $\tilde{F}_{n,\mu} = F_{n,\mu}^{(N_\rho)}$ for the smeared link $\tilde{U}_{n,\mu} = U_{n,\mu}^{(N_\rho)}$ is straightforward. Once we obtain the initial drift force $\tilde{F}_{n,\mu}$, the subsequent ones are given by the map from $F_{n,\mu}^{(k)}$ to $F_{n,\mu}^{(k-1)}$ iteratively.

$$\tilde{F}_{n,\mu} = F_{n,\mu}^{(N_\rho)} \rightarrow F_{n,\mu}^{(N_\rho-1)} \rightarrow \dots \rightarrow F_{n,\mu}^{(0)} = F_{n,\mu} \quad (22)$$

The map of the drift force is given by the following formulae, where the final step from $F'_{n,\mu} = F_{n,\mu}^{(1)}$ to $F_{n,\mu} = F_{n,\mu}^{(0)}$ is shown as an example.

$$F_{n,\mu} = e^{-iY_{n,\mu}} F'_{n,\mu} e^{iY_{n,\mu}} + \rho \text{Tr} \left[(U_{n,\mu} M_{n,\mu} + \bar{M}_{n,\mu} U_{n,\mu}^{-1}) \tau^a \right] \tau^a \quad (23)$$

$$\begin{aligned} M_{n,\mu} = & -\Omega_{n,\mu} \Lambda_{n,\mu} \\ & + \sum_{\nu(\neq\mu)} \left[U_{n+\hat{\mu},\nu} U_{n+\hat{\nu},\mu}^{-1} (U_{n,\nu}^{-1} \Lambda_{n,\nu} + \Lambda_{n+\hat{\nu},\mu} U_{n,\nu}^{-1}) \right. \\ & \quad + U_{n+\hat{\mu}-\hat{\nu},\nu}^{-1} U_{n-\hat{\nu},\mu}^{-1} (\Lambda_{n-\hat{\nu},\mu} - \Lambda_{n-\hat{\nu},\nu}) U_{n-\hat{\nu},\nu} \\ & \quad \left. - \Lambda_{n+\hat{\mu},\nu} U_{n+\hat{\nu},\mu} U_{n+\hat{\mu},\nu}^{-1} U_{n,\nu}^{-1} + U_{n+\hat{\mu}-\hat{\nu},\nu}^{-1} \Lambda_{n+\hat{\mu}-\hat{\nu},\nu} U_{n-\hat{\nu},\mu}^{-1} U_{n-\hat{\nu},\nu} \right] \end{aligned} \quad (24)$$

$$\begin{aligned} \bar{M}_{n,\mu} = & -\Lambda_{n,\mu} \bar{\Omega}_{n,\mu} \\ & + \sum_{\nu(\neq\mu)} \left[(\Lambda_{n,\nu} U_{n,\nu} + U_{n,\nu} \Lambda_{n+\hat{\nu},\mu}) U_{n+\hat{\nu},\mu} U_{n+\hat{\mu},\nu}^{-1} \right. \\ & + U_{n-\hat{\nu},\nu}^{-1} (\Lambda_{n-\hat{\nu},\mu} - \Lambda_{n-\hat{\nu},\nu}) U_{n-\hat{\nu},\mu} U_{n+\hat{\mu}-\hat{\nu},\nu} \\ & \left. - U_{n,\nu} U_{n+\hat{\nu},\mu} U_{n+\hat{\mu},\nu}^{-1} \Lambda_{n+\hat{\mu},\nu} + U_{n-\hat{\nu},\nu}^{-1} U_{n-\hat{\nu},\mu} \Lambda_{n+\hat{\mu}-\hat{\nu},\nu} U_{n+\hat{\mu}-\hat{\nu},\nu} \right] \end{aligned} \quad (25)$$

$$\Lambda_{m,\nu} = \text{Tr} [\hat{\Lambda}_{m,\nu} \tau^b] \tau^b \quad (26)$$

$$\hat{\Lambda}_{m,\nu} = -\frac{1}{2\kappa_{m,\nu}^2} \left(1 - \frac{\sin 2\kappa_{m,\nu}}{2\kappa_{m,\nu}} \right) \text{Tr} [F'_{m,\nu} iY_{m,\nu}] iY_{m,\nu} + \frac{\sin \kappa_{m,\nu}}{\kappa_{m,\nu}} e^{-iY_{m,\nu}} F'_{m,\nu} \quad (27)$$

$$\kappa_{n,\mu} = \sqrt{-\det Y_{n,\mu}} \quad (28)$$

Note that $Y_{n,\mu}$, $\Omega_{n,\mu}$ and $\bar{\Omega}_{n,\mu}$ are defined by (15), (17) and (18) respectively. They are calculated from $U_{n,\mu}$ in this case. The drift term calculated in this way respects the holomorphicity. The calculation time and the memory size required for the simulation are proportional to the number of steps N_ρ .

5. Result of the CLM

In this section, we show the results of the complex Langevin simulation. So far, we have found that the CLM using the naive definition (7) of the topological charge without the smearing works in the high-temperature region (deconfined phase). As a first step, we focus on the high-temperature region and try to see the effect of the stout smearing on the topological charge.

Before introducing the theta term, we check the effect of the smearing by changing the smearing parameters for $\theta = 0$. The number of steps N_ρ and the step size ρ should be large enough to eliminate the short range fluctuations. However, it is difficult to increase N_ρ a lot since the calculation time and the memory size increase with N_ρ . If ρ is too large, the nontrivial topological excitation will be destroyed. For $\beta > 2.4$, which corresponds to the high-temperature region in our setup, we find that $N_\rho = 20$ is enough to recover the topological property. In figure 1, we show the history of the topological charge defined by (19) in the real Langevin simulation for $\theta = 0$. There are three series of data with $\rho = 0, 0.06$ and 0.1 . We plot the topological charge without the smearing namely $\rho = 0$ for comparison. The topological charge with $\rho = 0$ is noisy, and it is difficult to see the topological property. Once we introduce the smearing, we can see the transitions between the topological sectors clearly.

Next, we show the results of the complex Langevin simulation for $\theta = \pi/4$. In this simulation, the lattice size is $24^3 \times 4$, and the smearing parameters are $N_\rho = 20$ and $\rho = 0.06$. In figure 2, we show the histogram of the magnitude u of the largest drift term defined in (12). The distribution falls off rapidly for $\beta = 2.55$, but it does not for $\beta = 2.5$. Thus, the criterion for correct convergence is satisfied only for $\beta = 2.55$. Typically, the coupling constant β should be large enough to satisfy the criterion. We found that the CLM works if $\beta \gtrsim 2.55$ for $\theta = \pi/4$ on the $24^3 \times 4$ lattice.

In figure 3, we show the history of the topological charge for $\beta = 2.55$. Since the gauge group is extended to $\text{SL}(2, \mathbb{C})$ in the CLM, the topological charge has an imaginary part in general. We plot both of the real part and the imaginary part. There are some topological excitations in the history of

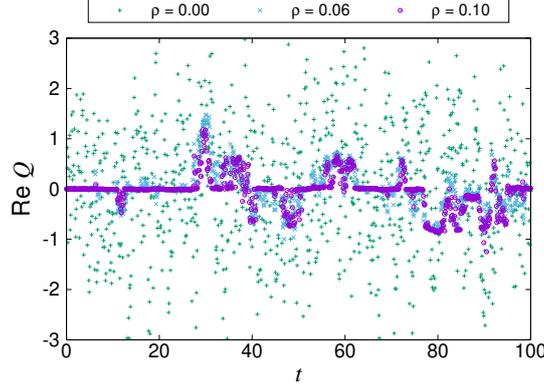


Figure 1: The history of the topological charge defined by (19) in the Langevin simulation for $\theta = 0$. The lattice size is $24^3 \times 4$, and the coupling constant is $\beta = 2.5$. The horizontal axis is the fictitious time t of the Langevin simulation.

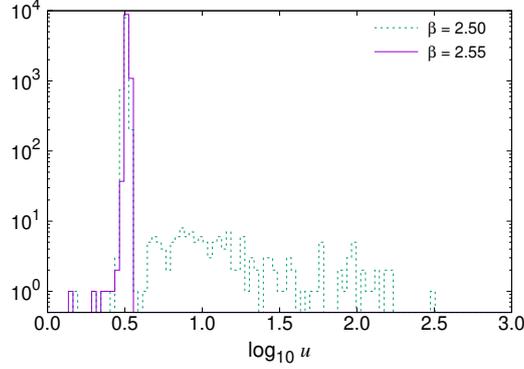


Figure 2: The histogram of the maximum drift term (12) for $\theta = \pi/4$ in log scale. The horizontal axis is $\log_{10} \mu$. The lattice size is $24^3 \times 4$, and the smearing parameters are $N_\rho = 20$ and $\rho = 0.06$.

$\text{Re}Q$. The imaginary part vanishes after the smearing in most cases, but it increases rapidly when the real part changes.

The expectation value of the topological charge has a nonzero imaginary part if CP is broken. Since the theta term breaks CP explicitly for $\theta/\pi \notin \mathbb{Z}$, it is consistent that $\text{Im}Q$ becomes nonzero in our simulation. We find that the fluctuation of $\text{Re}Q$ is necessary to obtain the nonzero $\text{Im}Q$. Indeed, the imaginary part are close to zero while the configuration stays in a single topological sector.

We also find that the rapid growth of $\text{Im}Q$ makes the simulation unstable. The imaginary part originates from the non-unitarity of the configuration, which can be a source of the large drift. We need to set β large enough to avoid this problem. However, the fluctuation of Q is highly suppressed for larger β , and the autocorrelation time of Q becomes longer than the simulation time. It is known as freezing of the topological charge, which causes a problem with the ergodicity. Therefore, it is difficult to avoid the large drift simply by increasing β further.

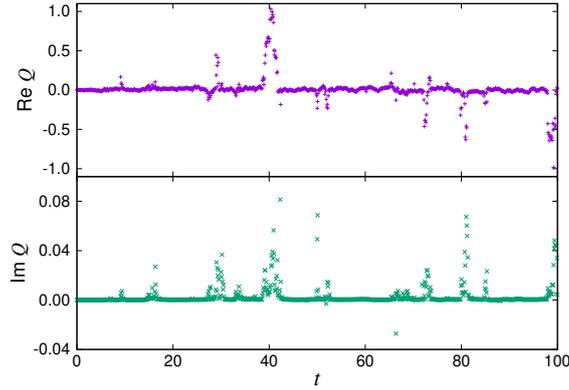


Figure 3: The history of the topological charge for $\theta = \pi/4$. The upper plot show the real part and the lower plot show the imaginary part. The lattice size is $24^3 \times 4$, and the coupling constant is $\beta = 2.55$. The horizontal axis is the fictitious time t of the Langevin simulation.

6. Summary

The sign problem prevents us from studying gauge theories with a theta term by the Monte Carlo simulation. In this work, we applied the complex Langevin method (CLM) to 4D SU(2) gauge theory to avoid the problem. We found that the criterion for correct convergence of the CLM is satisfied in the high temperature region. However, the naively defined topological charge does not take integer values due to the contamination by short range fluctuations. For this reason, we introduce the stout smearing in the CLM in order to recover the topological property. The effect of the smearing can be included in the Langevin dynamics itself as well as in observables. We confirmed that the real part of the topological charge becomes close to an integer after the smearing. On the other hand, the imaginary part vanishes mostly, but it grows rapidly as the real part changes. This behavior is consistent with the topological nature of the theory, although it is difficult to deal with in the numerical simulation.

We need to increase β to suppress the large drift. On the other hand, we cannot increase it due to the topology freezing. It seems to be necessary to resolve either of the topology freezing or the large drift in the CLM. However, it is possible that the appearance of large drift is related to the topology change, as we found in our previous study of 2D U(1) gauge theory [13]. In that case, we need to modify the boundary condition or try some possible ways to suppress the large drifts, such as improving the gauge cooling or the smearing method.

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