A practical solution to the sign problem at finite theta-vacuum angle

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We propose a practical way of circumventing the sign problem in lattice QCD simulations with a theta-vacuum term. This method is the reweighting method for the QCD Lagrangian after the $U_A(1)$ transformation. In the Lagrangian, the $P$-odd mass term as a cause of the sign problem is minimized. In order to find out a good reference system in the reweighting method, we estimate the average reweighting factor by using the two-flavor NJL model and eventually find a good reference system.

I. INTRODUCTION

Phenomena based on strong interaction have shown that charge conjugation $C$, parity $P$ and time reversal $T$ are good symmetries of nature. This means that quantum chromodynamics (QCD) should respect any combinations of the discrete symmetries. Among the discrete symmetries, the $CP$ symmetry is not necessarily respected in QCD due to the instanton solution [1,2]. The instanton solution allows the QCD dynamics (QCD) should respect any combinations of the discrete symmetries of nature. This means that quantum chromodynamics is the field strength of gluon. The vacuum angle $\theta$ is a periodic variable with period $2\pi$. It was known to be an observable parameter [3]. The Lagrangian $\mathcal{L}_{QCD}$ is invariant under the combination of the $P$ transformation and the parameter transformation $\theta \rightarrow -\theta$, indicating that the $P$ and $CP$ symmetries are preserved only at $\theta = 0$ and $\pm 2\pi$; note that $\theta = -\pi$ is identical with $\theta = \pi$. In the vacuum, therefore, we must consider the $P$ and $CP$ violating interaction parameterized by $\theta$. Theoretically we can take any arbitrary value between $-\pi$ and $\pi$ for $\theta$. Nevertheless, it has been found from the measured neutron electric dipole moment [4] that $|\theta| < 10^{-9}$ [5,6]. Why is $\theta$ so small in zero temperature ($T$)? This long-standing puzzle is called the strong $CP$ problem; see for example Ref. [8] for the review.

Around the deconfinement transition at $T = T_d$, there is a possibility that $P$-odd bubbles (metastable states) arise and thereby regions of nonzero $\theta$ are generated [9]. Thus $\theta$ can become a function depending on spacetime coordinates $(t, x)$. If $P$-odd bubbles are really produced at $T \approx T_{QCD}$, $P$ and $CP$ symmetries can be violated locally in high-energy heavy-ion collisions or the early universe. This finite value of $\theta$ could be a new source of large $CP$ violation in the early universe and a crucial missing element for solving the puzzle of baryogenesis.

In the early stage of heavy-ion collision, the magnetic field is formed, and simultaneously the total number of particles plus antiparticles with right-handed helicity is deviated from that with left-handed helicity by the effective $\theta(t, x)$. In this situation, particles with right-handed helicity move opposite to antiparticles with right-handed helicity, and consequently an electromagnetic current is generated along the magnetic field. This is the so-called chiral magnetic effect [10–13]. The chiral magnetic effect may explain the charge separations observed in the recent STAR results [14]. Hot QCD with nonzero $\theta$ is thus quite interesting.

For zero $T$ and zero quark-number chemical potential ($\mu$), some important properties are showed on $P$ symmetry. Vafa and Witten proved for $\theta = 0$ that the vacuum is unique and conserves $P$ symmetry [15]. This theorem does not preclude the existence of $P$-odd bubbles. At $\theta = \pi$, $P$ symmetry is also preserved as mentioned above, but it is spontaneously broken [16,17]. The spontaneous violation of $P$ symmetry is called the Dashen mechanism [16]. Although the mechanism is a nonperturbative phenomenon, the first-principle lattice QCD (LQCD) is not applicable for finite $\theta$ due to the sign problem. The mechanism at finite $T$ and/or finite $\mu$ was then investigated with effective models such as the chiral perturbation theory [18–23], the Nambu-Jona-Lasinio (NJL) model [24–27] and the Polyakov-loop extended Nambu-Jona-Lasinio (PNJL) model [28–30].

In the previous work [30], we proposed a way of minimizing the sign problem on LQCD with finite $\theta$. The proposal is as follows. For simplicity, we consider two-flavor QCD. The QCD Lagrangian (1) is transformed into

$$\mathcal{L}_{QCD} = \bar{q}_f (\gamma_\mu D_\mu + m_f) q_f + \frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu}$$

(1)

$$\mathcal{M}(\theta) = \gamma_\mu D_\mu + m \cos(\theta/2) + mi\gamma_5 \sin(\theta/2)$$

(3)

by using the $U_A(1)$ transformation

$$q = e^{i\gamma_5 \frac{\theta}{2}} q'$$

(4)
Fermion determinant of the reference theory that has no sign change as reference $A$ in this paper. As discussed, it is hard for LQCD simulations to reach.

We then propose the following reweighting method. The vacuum expectation value of operator $\mathcal{O}$ is calculated by

$$
\langle \mathcal{O} \rangle = \int D\mathcal{O} \det \mathcal{M}(\theta) e^{-S_g}
$$

with the gluon part $S_g$ of the QCD action and

$$
\mathcal{O}' \equiv R(\theta) \mathcal{O},
$$

$$
R(\theta) \equiv \frac{\det \mathcal{M}(\theta)}{\det \mathcal{M}_{\text{ref}}(\theta)},
$$

where $R(\theta)$ is the reweighting factor and $\det \mathcal{M}_{\text{ref}}(\theta)$ is the Fermion determinant of the reference theory that has no sign problem. The simplest candidate of the reference theory is the theory in which the $\theta$-odd mass is neglected. We refer this reference theory to as reference $A$ in this paper. As discussed in Ref. [30], reference $A$ may be a good reference theory for small and intermediate $\theta$, but not for large $\theta$ near $\pi$. In reference $A$, the limit of $\theta = \pi$ corresponds to the chiral limit that is hard for LQCD simulations to reach.

The expectation value of $\langle R(\theta) \rangle$ in the reference theory is obtained by

$$
\langle R(\theta) \rangle = \frac{Z}{Z_{\text{ref}}}
$$

where $Z$ ($Z_{\text{ref}}$) is the partition function of the original (reference) theory. The average reweighting factor $\langle R(\theta) \rangle$ is a good index for the reference theory to be good; the reference theory is good when $\langle R(\theta) \rangle = 1$.

In this paper, we estimate $\langle R(\theta) \rangle$ with the NJL model in order to find out a good reference theory. We find that reference $A$ is good only for small, so propose a good reference theory that satisfies $\langle R(\theta) \rangle \approx 1$.

This paper is organized as follows. In Sec. [III] we recapitulate the two-flavor NJL model and show how to calculate the pion mass and $\langle R(\theta) \rangle$ for the case of finite $\theta$. Numerical results are shown in Sec. [III] Section [IV] is devoted to summary.
where the momentum integral is regularized by the three-dimensional momentum cutoff $\Lambda$. Following Refs. [25,26], we introduce a parameter $c$ as $G_1 = (1 - c)G_+$ and $G_2 = cG_+$, where $0 \leq c \leq 0.5$ and $G_+ > 0$. The present model thus has four parameters of $m_0$, $\lambda$, $G_+$ and $c$. Assuming $m_0 = 5.5$ MeV, we have determined $\lambda$ and $G_+$ from the pion decay constant $f_\pi = 93$ MeV and the pion mass $\pi = 138$ MeV at vacuum. Although $c$ is an unknown parameter, we set $c = 0.2$ here, since it is known from the model analysis on the $\eta - \eta'$ splitting that $c \approx 0.2$ is favorable [32].

For finite $\theta$, parity is broken explicitly, so it is not a good quantum number anymore. Hence $P$-even and $P$-odd modes are mixed with each other for each meson. The "pion" mass $M_\pi$ is defined by the lowest pole mass of the inverse propagator in the isovector channel. It agrees with the ordinary mean-field level in the original (reference) theory and $\bar{c}$ is an unknown parameter, we set

\[ \beta V = 1 \]

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The right-hand side of (46) is reduced to
\[ \tilde{M}_\pi^2(\theta) = \frac{|\sigma_0|}{f^2} \left( m_0 \cos(\theta/2) + \frac{m_0 M_\pi^2}{M_{\eta'}^2} \sin^2(\theta/2) \right). \] (48)

Equation (48) supports (46).

### III. NUMERICAL RESULTS

If some reference system satisfies the condition that \( \langle R(\theta) \rangle \approx 1 \), one can say that the reference system is good. As a typical example of the condition, we consider the case of a threshold of \( 0.5 \lesssim \langle R(\theta) \rangle \lesssim 2 \). This condition seems to be the minimum requirement. The discussion made below is not changed qualitatively, even if one takes a stronger condition.

First we consider reference A. Figure 1(a) shows \( \theta \) dependence of \( \langle R(\theta) \rangle \) at \( T = 100 \text{ MeV} \). The solid line stands for \( \langle R(\theta) \rangle \), while the dashed (dotted) line corresponds to \( R_A \) (\( R_B \)). This temperature is lower than the chiral transition temperature in the original theory that is 206 MeV at \( \theta = 0 \) and 194 MeV at \( \theta = \pi \). As \( \theta \) increases from zero, \( \langle R(\theta) \rangle \) also increases and exceeds 2 at \( \theta \approx 1.2 \). Reference A is thus good for \( \theta \lesssim 1.2 \). The increase of \( \langle R(\theta) \rangle \) stems from that of \( R_B \) that depends on \( T \). This means that the reliable \( \theta \) region in which \( 0.5 \lesssim \langle R(\theta) \rangle \lesssim 2 \) becomes large as \( T \) increases.

Figure 1(b) shows \( \theta \) dependence of \( \tilde{M}_\pi \) at \( T = 100 \text{ MeV} \). The solid (dashed) line denotes \( \tilde{M}_\pi \) in the original (reference A) system. At \( \theta = \pi \), \( \tilde{M}_\pi \) is finite in the original system, but zero in reference A. As a consequence of this property, \( R_A \) and \( \langle R(\theta) \rangle \) vanish at \( \theta = \pi \); see Fig. 1(a). This indicates that reference A breaks down at \( \theta = \pi \), independently of \( T \).

The same analysis is made for reference B in Fig. 2. As shown in panel (b), \( \tilde{M}_\pi \) in reference B well reproduces that in reference B well reproduces that in reference A. Therefore reference B is still not good.

Finally we consider reference C. As shown in Fig. 3(b), \( \tilde{M}_\pi \) in reference C well reproduces that of the original theory for any \( \theta \). As shown in panel (a), however, the reliable \( \theta \) region in which \( 0.5 \lesssim \langle R(\theta) \rangle \lesssim 2 \) is located only at \( \theta \lesssim 1.3 \). Therefore reference B is still not good.

### IV. SUMMARY

We have proposed a practical way of circumventing the sign problem in LQCD simulations with finite \( \theta \). This method is the reweighting method for the transformed Lagrangian (2). In the Lagrangian, the sign problem is minimized, since the \( P \)-odd mass is much smaller than the dynamical quark mass of order \( \Lambda_{QCD} \). Another key is to find out which kind of reference system satisfies the condition \( \langle R(\theta) \rangle \approx 1 \). For this purpose, we have estimated \( \langle R(\theta) \rangle \) by using the two-flavor NJL model and eventually found that reference C is a good reference system for any \( \theta \). This is true for any temperature larger than 100 MeV.

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