Practical approach to the sign problem at finite theta-vacuum angle

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We investigate a way of circumventing the sign problem in lattice QCD simulations with a theta-vacuum term, using the Polyakov-loop extended Nambu–Jona-Lasinio model. We consider 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 a good reference system in the reweighting method, we estimate the average reweighting factor by using the two-flavor Polyakov-loop extended Nambu–Jona-Lasinio 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 $\mathcal{T}$ 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 Lagrangian $\mathcal{L}_{\rm QCD}$ to have a θ-vacuum term. The resulting Lagrangian is described as

$$\mathcal{L}_{\rm QCD} = \bar{q}_f(\gamma_\nu D_\nu + m_f)q_f + \frac{1}{4g^2}F_{\mu\nu}^a F_{\mu\nu}^a$$
$$- i\theta\frac{1}{64\pi^2}\epsilon_{\mu\nu\sigma\rho}F_{\mu\nu}^a F_{\sigma\rho}^a \qquad (1)$$

in Euclidean spacetime, where $F_{\mu\nu}^a$ is the field strength of the gluon. The vacuum angle θ is a periodic variable with period 2π. It was known to be an observable parameter [3]. The QCD Lagrangian is transformed as $\mathcal{L}_{\rm QCD}(\theta) \to \mathcal{L}_{\rm QCD}(-\theta)$ by the P transformation. Indicating that the P and CP symmetries are preserved only at $\theta = 0$ and $\pm\pi$, note that $\theta = -\pi$ is identical with $\theta = \pi$. In the θ vacuum, therefore, we must consider the P and CP violating interaction parameterized by θ. Theoretically, we can take any arbitrary value between $-\pi$ and π for θ. Nevertheless, it has been found from the measured neutron electric dipole moment [4] that $|\theta| < 10^{-9}$ [5–7]. Why is θ 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 θ are generated [9]. Thus θ can become a function depending on spacetime coordinates (t, x). If P-odd bubbles are really produced at

$T \approx \Lambda_{\rm QCD}$, P and CP symmetries can be violated locally in high-energy heavy-ion collisions or the early Universe. This finite value of θ 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 θ is thus quite interesting.

For zero T and zero quark-number chemical potential (μ), 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 $\theta = \pi$, QCD possesses P symmetry as mentioned above, but it is spontaneously broken at low T [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 θ due to the sign problem. The mechanism at finite T and/or finite μ 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]. LQCD has no sign problem at imaginary θ. Very recently, the region was analyzed with LQCD, and θ dependence of the deconfinement transition temperature was investigated [31].

In the previous work [30], we proposed a way of minimizing the sign problem on LQCD with finite θ. The proposal is as follows. For simplicity, we consider

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two-flavor QCD. The QCD Lagrangian (1) is transformed into

$$\mathcal{L}_{\text{QCD}} = \bar{q}'\mathcal{M}(\theta)q' + \frac{1}{4g^2}F^a_{\mu\nu}F^a_{\mu\nu} \qquad (2)$$

with

$$\mathcal{M}(\theta) \equiv \gamma_\nu D_\nu + m\cos(\theta/2) + mi\gamma_5\sin(\theta/2) \qquad (3)$$

by using the $U_A(1)$ transformation

$$q = e^{i\gamma_5\frac{\theta}{4}}q', \qquad (4)$$

where the quark field $q = (q_u, q_d)$ has been redefined by the new one q'. The determinant $\mathcal{M}(\theta)$ satisfies

$$\det \mathcal{M}(\theta) = [\det \mathcal{M}(-\theta)]^*, \qquad (5)$$

indicating that the sign problem is induced by the P-odd (θ-odd) term $mi\gamma_5\sin(\theta/2)$. The difficulty of the sign problem is minimized in (2), since the P-odd term with the light quark mass m is much smaller than the dynamical quark mass of order Λ_{QCD}. Actually, it was found that the P-even condensates $\sigma'_f = \langle\bar{q}'_f q'_f\rangle$ are much larger than the P-odd condensates $\eta'_f = \langle\bar{q}'_f i\gamma_5 q'_f\rangle$. The P-even condensates change little even if the θ-odd mass term is neglected. We then proposed the following reweighting method. The vacuum expectation value of operator $\mathcal{O}$ is calculated by

$$\langle\mathcal{O}\rangle = \int \mathcal{D}A\mathcal{O}\det\mathcal{M}(\theta)e^{-S_g} \qquad (6)$$

$$= \int \mathcal{D}A\mathcal{O}'\det\mathcal{M}_{\text{ref}}(\theta)e^{-S_g} \qquad (7)$$

with the gluon part S_g of the QCD action and

$$\mathcal{O}' \equiv R(\theta)\mathcal{O}, \qquad (8)$$

$$R(\theta) \equiv \frac{\det\mathcal{M}(\theta)}{\det\mathcal{M}_{\text{ref}}(\theta)}, \qquad (9)$$

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 θ-odd mass is neglected. We refer to this reference theory as reference A in this paper. As discussed in Ref. [30], reference A may be a good reference theory for small and intermediate θ, but not for large θ near π. 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 $R(\theta)$ in the reference theory is obtained by

$$\langle R(\theta)\rangle = \frac{Z}{Z_{\text{ref}}}, \qquad (10)$$

where Z (Z_{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 PNJL model in order to find a good reference theory. Lagrangian (2) does not depend on θ in the chiral limit. For the realistic case closer to this limit rather than the pure gauge limit, an effect of finite θ is characterized by the current quark mass. Hence, it is expected that the finite θ effect is well described by effective models such as the PNJL model. As shown in Sec. III, reference A is good only for small θ, so we propose the good reference theory that satisfies $\langle R(\theta)\rangle \approx 1$.

This paper is organized as follows. In Sec. II, we recapitulate the two-flavor PNJL model and show how to calculate the pion mass and $\langle R(\theta)\rangle$ for the case of finite θ. Numerical results are shown in Sec. III. Section IV is devoted to a summary.

II. MODEL SETTING

The two-flavor PNJL Lagrangian with the θ-dependent anomaly term is obtained in Euclidean spacetime by

$$\mathcal{L} = \bar{q}(\gamma_\nu D_\nu + m_0)q - G_1 \sum_{a=0}^{3}[(\bar{q}\tau_a q)^2 + (\bar{q}i\gamma_5\tau_a q)^2]$$
$$- 8G_2[e^{i\theta}\det\bar{q}_R q_L + e^{-i\theta}\det\bar{q}_L q_R] + \mathcal{U}(T, \Phi, \Phi^*),$$
$$(11)$$

where $D_\nu = \partial_\nu - i\delta_{\nu4}A^a_4/\lambda_a/2$ with the Gell-Mann matrices λ_a. The current quark mass m_0 satisfies $m_0 = m_u = m_d$, and τ_0 and $\tau_a(a = 1, 2, 3)$ are the 2×2 unit and Pauli matrices in the flavor space, respectively. The parameter G_1 denotes the coupling constant of the scalar and pseudoscalar-type four-quark interaction, while G_2 stands for that of the Kobayashi-Maskawa-'t Hooft determinant interaction [2,32] where the matrix indices run in the flavor space.

The gauge field A_μ is treated as a homogeneous and static background field in the PNJL model [28–30,33–39]. The Polyakov-loop Φ and its conjugate Φ^* are determined in the Euclidean space by

$$\Phi = \frac{1}{3}\text{tr}_c(L), \qquad \Phi^* = \frac{1}{3}\text{tr}_c(\bar{L}), \qquad (12)$$

where $L = \exp(iA_4/T)$ with $A_4/T = \text{diag}(\phi_r, \phi_g, \phi_b)$ in the Polyakov gauge; note that λ_a is traceless and hence $\phi_r + \phi_g + \phi_b = 0$. Therefore we obtain

$$\Phi = \frac{1}{3}(e^{i\phi_r} + e^{i\phi_g} + e^{i\phi_b})$$
$$= \frac{1}{3}(e^{i\phi_r} + e^{i\phi_g} + e^{-i(\phi_r+\phi_g)}),$$

$$\Phi^* = \frac{1}{3}(e^{-i\phi_r} + e^{-i\phi_g} + e^{-i\phi_b})$$
$$= \frac{1}{3}(e^{-i\phi_r} + e^{-i\phi_g} + e^{i(\phi_r+\phi_g)}). \qquad (13)$$

We use the Polyakov potential $\mathcal{U}$ of Ref. [37]:

$$\mathcal{U} = T^4 \left[-\frac{a(T)}{2} \Phi^* \Phi + b(T) \ln (1 - 6\Phi\Phi^* \right.$$
$$\left. + 4(\Phi^3 + \Phi^{*3}) - 3(\Phi\Phi^*)^2) \right] \qquad (14)$$

with

$$a(T) = a_0 + a_1 \left(\frac{T_0}{T}\right) + a_2 \left(\frac{T_0}{T}\right)^2, \qquad b(T) = b_3 \left(\frac{T_0}{T}\right)^3. \qquad (15)$$

The parameter set in $\mathcal{U}$ is fitted to LQCD data at finite T in the pure gauge limit. The parameters except T_0 are summarized in Table I. The Polyakov potential yields a first-order deconfinement phase transition at $T = T_0$ in the pure gauge theory. The original value of T_0 is 270 MeV determined from the pure gauge LQCD data, but the PNJL model with this value of T_0 yields a larger value of the pseudocritical temperature T_c of the deconfinement transition at zero chemical potential than $T_c \approx 173 \pm 8$ MeV predicted by full LQCD [40–42]. Therefore we rescale T_0 to 212 MeV so as to reproduce the LQCD result. Under the $U_A(1)$ transformation (4), the quark-antiquark condensates are transformed as

$$\sigma \equiv \bar{q}q = \cos(\theta/2)\sigma' + \sin(\theta/2)\eta', \qquad (16)$$

$$\eta \equiv \bar{q}i\gamma_5 q = -\sin(\theta/2)\sigma' + \cos(\theta/2)\eta', \qquad (17)$$

$$a_i \equiv \bar{q}\tau_i q = \cos(\theta/2)a_i' + \sin(\theta/2)\pi_i', \qquad (18)$$

$$\pi_i \equiv \bar{q}i\gamma_5\tau_i q = -\sin(\theta/2)a_i' + \cos(\theta/2)\pi_i', \qquad (19)$$

where the condensates $\{\sigma', \eta', a_i', \pi_i'\}$ are defined by the same form as $\{\sigma, \eta, a_i, \pi_i\}$ but q is replaced by q'. The Lagrangian density is then rewritten with q' as

$$\mathcal{L} = \bar{q}'(\gamma_\nu D_\nu + m(\theta))q' - G_1 \sum_{a=0}^{3} [(\bar{q}'\tau_a q')^2 + (\bar{q}'i\gamma_5\tau_a q')^2]$$
$$- 8G_2 [\det \bar{q}_R' q_L' + \det \bar{q}_L' q_R'] + \mathcal{U} \qquad (20)$$

$$= \bar{q}'(\gamma_\nu D_\nu + m(\theta))q' - G_+ [(\bar{q}'q')^2 + (\bar{q}'i\gamma_5\vec{\tau}q')^2]$$
$$- G_- [(\bar{q}'\vec{\tau}q')^2 + (\bar{q}'i\gamma_5 q')^2] + \mathcal{U}, \qquad (21)$$

where $G_\pm = G_1 \pm G_2$ and

TABLE I. Summary of the parameter set in the Polyakov-potential sector determined in Ref. [37]. All parameters are dimensionless.

a_0	a_1	a_2	b_3
3.51	-2.47	15.2	-1.75

$$m(\theta) = m_0 \cos(\theta/2) + m_0 i\gamma_5 \sin(\theta/2). \qquad (22)$$

Making the mean-field approximation and the path integral over the quark field, one can obtain the thermodynamic potential Ω (per volume) for finite T:

$$\Omega = U + \mathcal{U} - 2\sum_{\pm} \int \frac{d^3 p}{(2\pi)^3}$$
$$\times [3E_\pm + T\ln[1 + 3\Phi e^{-\beta E_\pm} + 3\Phi^* e^{-2\beta E_\pm} + e^{-3\beta E_\pm}]$$
$$+ T\ln[1 + 3\Phi^* e^{-\beta E_\pm} + 3\Phi e^{-2\beta E_\pm} + e^{-3\beta E_\pm}]] \qquad (23)$$

with

$$E_\pm = \sqrt{\vec{p}^2 + C \pm 2\sqrt{D}}, \qquad (24)$$

$$C = M^2 + N^2 + A^2 + P^2, \qquad (25)$$

$$D = (M\vec{A} + N\vec{P})^2 + (\vec{A} \times \vec{P})^2 \geq 0, \qquad (26)$$

$$M = m_0 \cos(\theta/2) - 2G_+ \sigma', \qquad (27)$$

$$N = m_0 \sin(\theta/2) - 2G_- \eta', \qquad (28)$$

$$\vec{A} = -2G_- \vec{a}', \qquad \vec{P} = -2G_+ \vec{\pi}', \qquad (29)$$

$$A = \sqrt{\vec{A} \cdot \vec{A}}, \qquad P = \sqrt{\vec{P} \cdot \vec{P}}, \qquad (30)$$

$$U = G_+(\sigma'^2 + \vec{\pi}'^2) + G_-(\eta'^2 + \vec{a}'^2), \qquad (31)$$

where the momentum integral is regularized by the three-dimensional momentum cutoff Λ. 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, λ, G_+, and c. Assuming $m_0 = 5.5$ MeV, we have determined Λ and G_+ from the pion decay constant $f_\pi = 93$ MeV and the pion mass $M_\pi = 138$ 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 [43].

For finite θ, 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 $\tilde{M}_\pi$ is defined by the lowest pole mass of the inverse propagator in the isovector channel. It agrees with the ordinary pion mass when $\theta = 0$. Under the random phase approximation [44], the inverse propagator is described by

$$\det [1 - 2G\Pi(\tilde{M}_\pi^2)] = 0, \qquad (32)$$

where

$$G = \begin{pmatrix} G_- & 0 \\ 0 & G_+ \end{pmatrix}, \qquad (33)$$

$$\Pi(\omega^2) = \begin{pmatrix} \Pi^{SS}(\omega^2) & \Pi^{SP}(\omega^2) \\ \Pi^{PS}(\omega^2) & \Pi^{PP}(\omega^2) \end{pmatrix} \qquad (34)$$

with

$$\Pi^{PP} = 4N_f N_c I_1 - 2N_f N_c (q^2 - 4N^2) I_2(\omega^2), \quad (35)$$

$$\Pi^{SS} = 4N_f N_c I_1 - 2N_f N_c (q^2 - 4M^2) I_2(\omega^2), \quad (36)$$

$$\Pi^{SP} = \Pi^{PS} = -8N_f N_c MN I_2(\omega^2), \qquad (37)$$

$$I_1 = \int_\Lambda \frac{d^3 p}{(2\pi)^3} \frac{1 - f_\Phi^+(E_p) - f_\Phi^-(E_p)}{2E_p}, \qquad (38)$$

$$I_2(\omega^2) = \int_\Lambda \frac{d^3 p}{(2\pi)^3} \frac{1 - f_\Phi^+(E_p) - f_\Phi^-(E_p)}{E_p(\omega^2 - 4E_p^2)}, \qquad (39)$$

and

$$f_\Phi^+ = \frac{(\Phi^* + 2\Phi e^{-\beta E_p}) e^{-\beta E_p} + e^{-3\beta E_p}}{1 + 3(\Phi^* + \Phi e^{-\beta E_p}) e^{-\beta E_p} + e^{-3\beta E_p}}, \quad (40)$$

$$f_\Phi^- = \frac{(\Phi + 2\Phi^* e^{-\beta E_p}) e^{-\beta E_p} + e^{-3\beta E_p}}{1 + 3(\Phi + \Phi^* e^{-\beta E_p}) e^{-\beta E_p} + e^{-3\beta E_p}}. \quad (41)$$

In this form, we can set $\vec{a}' = \vec{\pi}' = 0$, since we do not consider the isospin chemical potential.

Applying the saddle-point approximation to the path integral in the partition function, one can get

$$\langle R(\theta) \rangle \approx \sqrt{\frac{\det H_{\text{ref}}}{\det H}} e^{-\beta V(\Omega - \Omega_{\text{ref}})}, \qquad (42)$$

where $\beta = 1/T$, Ω (Ω_{ref}) is the thermodynamic potential of the original (reference) theory in the mean-field level, and H (H_{ref}) is the Hessian matrix in the original (reference) theory defined by [45,46]

$$H_{ij} = \frac{\partial^2 \Omega}{\partial \phi_i' \partial \phi_j'}, \qquad (43)$$

$$\{\phi_i\} = \{\sigma', \eta', a_i', \pi_i', \Phi, \Phi^*\}. \qquad (44)$$

For later convenience, the average reweighting factor $\langle R(\theta) \rangle$ is divided into two factors R_H and R_Ω:

$$\langle R(\theta) \rangle = R_H R_\Omega \qquad (45)$$

with

$$R_H = \sqrt{\frac{\det H_{\text{ref}}}{\det H}}, \qquad (46)$$

$$R_\Omega = e^{-\beta V(\Omega - \Omega_{\text{ref}})}. \qquad (47)$$

For an $N_x^3 \times N_\tau$ lattice, the four-dimensional volume βV is obtained by

$$\beta V = \left(\frac{N_x}{N_\tau}\right)^3 \frac{1}{T^4}. \qquad (48)$$

Here we consider $N_x/N_\tau = 4$ as a typical example, following Refs. [45,46].

We consider the following reference theory that has no sign problem:

$$\mathcal{L} = \bar{q}'(\gamma_\nu \partial_\nu + m_{\text{ref}}(\theta))q' - G_+[(\bar{q}'q')^2 + (\bar{q}'i\gamma_5\vec{\tau}q')^2]$$
$$- G_-[(\bar{q}'\vec{\tau}q')^2 + (\bar{q}'i\gamma_5 q')^2] + \mathcal{U}. \qquad (49)$$

Here $m_{\text{ref}}(\theta)$ is θ-even mass defined below. We consider three examples as $m_{\text{ref}}(\theta)$.

(A) The first example is reference A defined by

$$m_{\text{ref}}(\theta) \equiv m_A(\theta) = m_0 \cos(\theta/2). \qquad (50)$$

In this case, the P-odd mass is simply neglected from the original Lagrangian (21).

(B) The second example is reference B defined by

$$m_{\text{ref}}(\theta) \equiv m_B(\theta)$$
$$= m_0 \cos(\theta/2) + \frac{1}{\alpha}\{m_0 \sin(\theta/2)\}^2. \quad (51)$$

In this case, we have added the m_0^2-order correction due to the P-odd quark mass. Here α is a parameter with mass dimension, so we simply choose $\alpha = M_\pi$. The coefficient of the correction term is $m_0^2/M_\pi = 0.129$ MeV.

(C) The third case is reference C defined by

$$m_{\text{ref}}(\theta) \equiv m_C(\theta)$$
$$= m_0 \cos(\theta/2) + \frac{m_0 M_\pi^2}{M_{\eta'}^2} \sin^2(\theta/2). \quad (52)$$

This case also has the m_0^2-order correction, but α is different from reference B. The coefficient of the correction term is $m_0 M_\pi^2/M_{\eta'}^2 = 0.114$ MeV.

Reference C is justified as follows. The pion mass $\tilde{M}_\pi(\theta)$ at finite θ is estimated from the chiral Lagrangian as [23]

$$\tilde{M}_\pi^2(\theta) = \frac{m_0|\sigma_0|}{f_\pi^2}|\cos(\theta/2)| + \frac{2l_7 m_0^2 \sigma_0^2}{f_\pi^6} \sin^2(\theta/2), \quad (53)$$

where σ_0 is the chiral condensate at $T = \theta = 0$ and the coefficient l_7 is evaluated by the $1/N_c$ expansion as

$$l_7 \approx \frac{f_\pi^2}{2M_{\eta'}^2}. \qquad (54)$$

The right-hand side of (53) is reduced to

$$\tilde{M}_\pi^2(\theta) = \frac{|\sigma_0|}{f_\pi^2}\left[m_0|\cos(\theta/2)| + \frac{m_0 M_\pi^2}{M_{\eta'}^2}\sin^2(\theta/2) \right]. \quad (55)$$

Equation (55) supports (52).

III. NUMERICAL RESULTS

A. Mean-field approximation

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 $0.5 \lesssim \langle R(\theta)\rangle \lesssim 2$. 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 θ dependence of $\langle R(\theta)\rangle$ at $T = 100$ MeV. The solid line stands for $\langle R(\theta)\rangle$, while the dashed (dotted) line corresponds to R_H (R_Ω). This temperature is lower than the chiral transition temperature in the original theory, that is, 212 MeV at $\theta = 0$ and 204 MeV at $\theta = \pi$. As θ 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_Ω that depends on T. This means that the reliable θ region in which $0.5 \lesssim \langle R(\theta)\rangle \lesssim 2$ becomes large as T increases.

Figure 1(b) shows θ dependence of $\tilde{M}_\pi$ at $T = 100$ 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_H 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. $\tilde{M}_\pi$ in reference B well reproduces that in the original theory for any θ, and $\langle R(\theta)\rangle$ satisfies the condition $0.5 \lesssim \langle R(\theta)\rangle \lesssim 2$ for all θ. Since $R_H \sim 1$ in the most region of θ, $\langle R(\theta)\rangle$ is governed by R_Ω. Around $\theta = \pi$, R_H becomes small but still has a nonzero value because $\tilde{M}_\pi \neq 0$ even at $\theta = \pi$ in reference B. Therefore, the simple estimation for $m_{\text{ref}}(\theta)$ (51) gives an available reference.

Finally, we consider reference C through Fig. 3. $\tilde{M}_\pi$ in reference C well simulates that in the original theory, and $\langle R(\theta)\rangle$ satisfies the condition $0.5 \lesssim \langle R(\theta)\rangle \lesssim 2$ for all θ. This result is better than that in reference B. Therefore we can think that reference C is a good reference system for any θ. This is true for any temperature larger than 100 MeV.

B. Effect of mesonic fluctuation

Beyond the mean-field approximation, we estimate an effect of dynamical pion fluctuations by modifying the thermodynamic potential to

$$\Omega = \Omega_{\text{MF}} + \Omega_{\text{DF}}, \quad (56)$$

where Ω_{MF} is the thermodynamic potential (23) with the mean-field level. Ω_{DF} is the potential due to dynamical pion fluctuations [46],
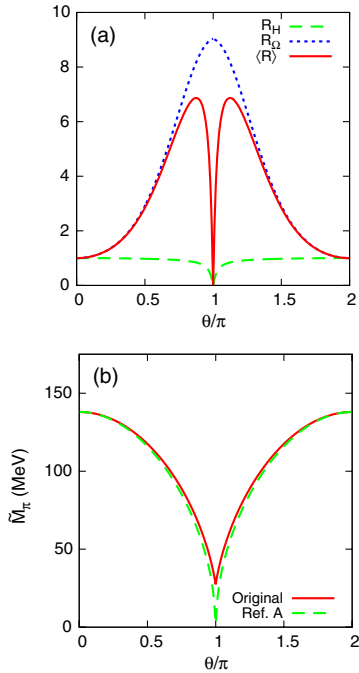

FIG. 1 (color online). θ dependence of (a) the average reweighting factor and (b) $\tilde{M}_\pi$ at $T = 100$ MeV for the case of reference A.
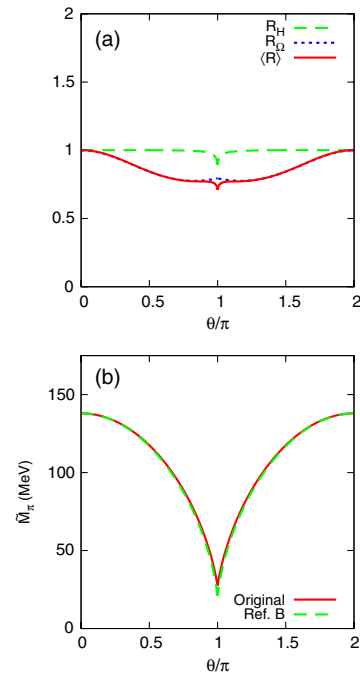

FIG. 2 (color online). θ dependence of (a) the average reweighting factor and (b) $\tilde{M}_\pi$ at $T = 100$ MeV for the case of reference B.
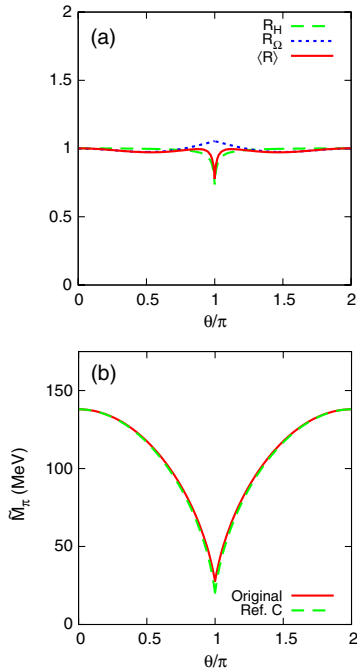
FIG. 3 (color online). θ dependence of (a) the average reweighting factor and (b) $\tilde{M}_\pi$ at $T = 100$ MeV for the case of reference C.

$$\Omega_{\mathrm{DF}} = 3 \int \frac{d^3 p}{(2\pi)^3} T \ln (1 - e^{-\beta E_\pi}), \qquad (57)$$

where $E_\pi = \sqrt{\vec{p}^2 + \tilde{M}_\pi^2}$, with $\tilde{M}_\pi$ determined by solving (32).

Figure 4 shows θ dependence of $\langle R(\theta) \rangle$ at $T = 100$ MeV for the case of reference C. The solid and dashed lines correspond to results with and without dynamical pion fluctuations, respectively. The effect makes $\langle R \rangle$ a little smaller, and hence reference C becomes slightly worse. However, the modification is small, indicating that $\langle R \rangle$ is well evaluated by the mean-field approximation.

IV. SUMMARY AND DISCUSSION

We have investigated a way of circumventing the sign problem in LQCD simulations with finite θ, using the PNJL model. We have considered the reweighting method for the transformed Lagrangian (2). In the Lagrangian, the
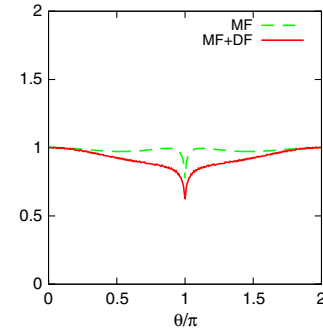

FIG. 4 (color online). θ dependence of the average reweighting factor at $T = 100$ MeV for the case of reference C. Solid and dashed lines correspond to the result with and without dynamical pion fluctuation, respectively.

sign problem is minimized, since the P-odd mass is much smaller than the dynamical quark mass of order Λ_{QCD}. Another key is which kind of reference system satisfies the condition $\langle R(\theta) \rangle \approx 1$. We have then estimated $\langle R(\theta) \rangle$ by using the two-flavor PNJL model and have found that reference C may be a good reference system in the reweighting method.

Since the present proposal is based on the model analysis, it is then not obvious whether the proposal really works in lattice simulations. Therefore, the proposal should be directly tested by lattice simulations. A similar test was made for two-flavor QCD with finite quark chemical potential μ [46,47] where lattice simulations have the sign problem. The average reweighting factor, i.e., the average phase factor, was evaluated by lattice simulations at $\mu/T < 1$ for T around the critical temperature of the deconfinement transition [47]. The PNJL model well reproduces the lattice result, when the dynamical correction due to mesonic fluctuations is made to the mean-field model calculation [46]. It is thus interesting that the present proposal is directly tested by lattice simulations.

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