Meson mass and the sign problem at finite theta

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Abstract. We propose a practical way of circumventing the sign problem in lattice QCD simulations with the theta-vacuum term. This method is the reweighting method for QCD Lagrangian after the $U_{\rm A}(1)$ 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.

1. Introduction

The existence of instanton solution requires QCD Lagrangian with the theta vacuum:

$$\mathcal{L} = \sum_f \bar{q}_f(\gamma_\nu D_\nu + m_f)q_f + \frac{1}{4g^2}F^a_{\mu\nu}F^a_{\mu\nu} - i\theta\frac{1}{64\pi^2}\varepsilon_{\mu\nu\sigma\rho}F^a_{\mu\nu}F^a_{\sigma\rho}, \tag{1}$$

in Euclidean spacetime. Hereafter, we will consider two-flavor QCD and assume isospin symmetry, $m_u = m_d = m_0$. Though the angle θ can take any arbitrary value theoretically, experimental measurements of neutron dipole moment give the upper limit, $|\theta| < 10^{-9}$[1, 2]. Why should θ be so small? This long-standing puzzle is called the strong CP problem.

Since the upper limit is determined only at zero temperature, the behavior is nontrivial for finite temperature. Hence the first-principle lattice simulation is needed, but it has the sign problem for finite θ. After making $U_A(1)$ transformation

$$q = e^{i\gamma_5\frac{\theta}{4}}q', \tag{2}$$

θ dependence appears only through the mass term

$$m_0(\theta) = m_0\cos(\theta/2) + m_0 i\gamma_5\sin(\theta/2), \tag{3}$$

in the transformed Lagrangian

$$\mathcal{L} = \sum_f \bar{q}_f(\gamma_\nu D_\nu + m_0(\theta))q_f + \frac{1}{4g^2}F^a_{\mu\nu}F^a_{\mu\nu}. \tag{4}$$

The P-odd mass term including $i\gamma_5$ makes the fermion determinant complex.

Because of the sign problem, we should perform a reweighting method in lattice simulations. The vacuum expectation value of operator $\mathcal{O}$ is obtained by

$$\langle\mathcal{O}\rangle = \int \mathcal{D}A\mathcal{O}\mathrm{det}\mathcal{M}(\theta)e^{-S_g} \tag{5}$$

$$= \int \mathcal{D}A\mathcal{O}'\mathrm{det}\mathcal{M}_{\mathrm{ref}}(\theta)e^{-S_g} \tag{6}$$

with the gluon part S_g of the QCD action and

$$\mathcal{O}' \equiv R(\theta)\mathcal{O}, \tag{7}$$

$$R(\theta) \equiv \frac{\mathrm{det}\mathcal{M}(\theta)}{\mathrm{det}\mathcal{M}_{\mathrm{ref}}(\theta)}, \tag{8}$$

where $R(\theta)$ is the reweighting factor and $\det \mathcal{M}_{\mathrm{ref}}(\theta)$ 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 term is neglected in the mass term (3). We refer to this reference theory as reference A in this paper. As discussed in Ref. [3], 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 for $\mathrm{det}\mathcal{M}_{\mathrm{ref}}$ that is hard for LQCD simulations to reach.

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

$$\langle R(\theta)\rangle = \frac{Z}{Z_{\mathrm{ref}}} \tag{9}$$

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 two-flavor NJL model in order to find out a good reference theory. We find that reference A is good only for small θ, so propose a good reference theory that satisfies $\langle R(\theta)\rangle \approx 1$. This work is based on the Ref. [4].

2. Model setting

The two-flavor NJL Lagrangian with the θ-dependent term is obtained by

$$\mathcal{L} = \bar{q}(\gamma_\nu\partial_\nu + m_0)q - G_1\sum_{a=0}^{3}\left[(\bar{q}\tau_a q)^2 + (\bar{q}i\gamma_5\tau_a q)^2\right] - 8G_2\left[e^{i\theta}\mathrm{det}\bar{q}_{\mathrm{R}}q_{\mathrm{L}} + e^{-i\theta}\mathrm{det}\bar{q}_{\mathrm{L}}q_{\mathrm{R}}\right], \tag{10}$$

in Euclidean spacetime where m_0 is the current quark mass 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 interactions, while G_2 stands for that of the Kobayashi-Maskawa-'t Hooft determinant interaction [5, 6] where the matrix indices run in the flavor space. Under the $U_A(1)$ transformation (2), the Lagrangian density is then rewritten with q' as

$$\mathcal{L} = \bar{q}'(\gamma_\nu\partial_\nu + m_0(\theta))q' - G_+\left[(\bar{q}'q')^2 + (\bar{q}'i\gamma_5\vec{\tau}q')^2\right] - G_-\left[(\bar{q}'\vec{\tau}q')^2 + (\bar{q}'i\gamma_5 q')^2\right], \tag{11}$$

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

Applying the saddle-point approximation to the path integral in the partition function, one can get the average reweighting factor $\langle R(\theta)\rangle$,

$$\langle R(\theta)\rangle \approx R_A R_B \tag{12}$$

$$R_A = \sqrt{\frac{\mathrm{det}H_{\mathrm{ref}}}{\mathrm{det}H}} \quad , \quad R_B = e^{-\beta V(\Omega-\Omega_{\mathrm{ref}})}, \tag{13}$$

where $\beta = 1/T$ and Ω ($\Omega_{\rm ref}$) is the thermodynamic potential at the mean-field level in the original (reference) theory [4]. H ($H_{\rm ref}$) is the Hessian matrix in the original (reference) theory defined by [7, 8]

$$H_{ij} = \frac{\partial^2 \Omega}{\partial \phi'_i \partial \phi'_j} , \quad \{\phi'_i\} = \{\sigma', \eta', \vec{a}', \vec{\pi}'\}, \tag{14}$$

with the quark-condensates

$$\sigma' = \langle \bar{q}q \rangle \ , \quad \eta' = \langle \bar{q}i\gamma_5 q \rangle \ , \quad \vec{a}' = \langle \bar{q}\vec{\tau}q \rangle \ , \quad \vec{\pi}' = \langle \bar{q}i\gamma_5\vec{\tau}q \rangle \, . \tag{15}$$

The four-dimensional volume βV is obtained by $\beta V = (N_x/N_\tau)^3 T^{-4}$ for the $N_x^3 \times N_\tau$ lattice. Here we consider $N_x/N_\tau = 4$ as a typical example, following Refs. [7, 8].

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

$$\mathcal{L} = \bar{q}'(\gamma_\nu \partial_\nu + m_{\rm ref}(\theta))q' - G_+ \left[(\bar{q}'q')^2 + (\bar{q}'i\gamma_5\vec{\tau}q')^2\right] - G_- \left[(\bar{q}'\vec{\tau}q')^2 + (\bar{q}'i\gamma_5 q')^2\right] . \tag{16}$$

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

3. Numerical results

If some reference system satisfies the condition $\langle R(\theta)\rangle \approx 1$, 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.

The first example is reference A defined by

$$\begin{aligned} m_{\rm ref}(\theta) &\equiv m_{\rm A}(\theta) \\ &= m_0 \cos(\theta/2). \end{aligned} \tag{17}$$

In this case, the P-odd mass is simply neglected from the original Lagrangian (11).

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 $R_{\rm A}$ ($R_{\rm B}$). 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 θ increases from zero, $\langle R(\theta)\rangle$ also increases and exceeds 2 at $\theta \approx 1.2$. Reference A is thus good for $\theta \lesssim 1.2$.

Figure 1(b) shows θ dependence of pion mass $\tilde{M}_\pi$ at $T = 100$ MeV. Since P symmetry is broken at finite θ, P-even modes and P-odd modes are mixed with each other for each meson. Hence, $\tilde{M}_\pi$ is defined by the lowest pole mass of the inverse propagator in the isovector channel[4]. 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, $R_{\rm A}$ and $\langle R(\theta)\rangle$ vanish at $\theta = \pi$; see Fig. 1(a). This indicates that reference A breaks down at $\theta = \pi$.

The second example is reference B defined by

$$\begin{aligned} m_{\rm ref}(\theta) &\equiv m_{\rm B}(\theta) \\ &= m_0 \cos(\theta/2) + \frac{1}{\alpha}\left\{m_0 \sin(\theta/2)\right\}^2 . \end{aligned} \tag{18}$$

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.

The same analysis is made for reference B in Fig. 2. As shown in panel (b), $\tilde{M}_\pi$ in reference

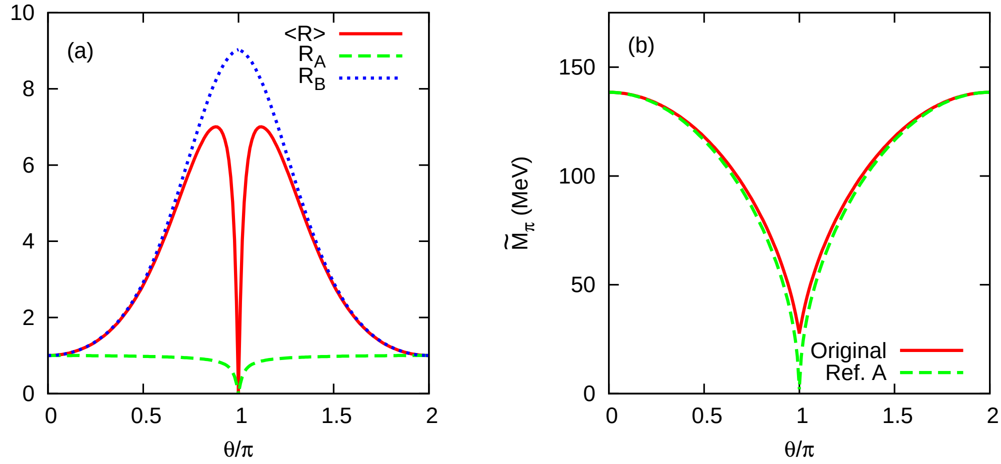

Figure 1. θ dependence of (a) the average reweighting factor and (b) $\tilde{M}_\pi$ at $T = 100$ MeV for the case of reference A.

B well reproduces that in the original theory for any θ. As shown in panel (a), however, the reliable θ 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.

Finally we consider reference C. The pion mass $\tilde{M}_\pi(\theta)$ at finite θ is estimated from the chiral Lagrangian and $1/N_c$ analysis [9]:

$$\tilde{M}_\pi^2(\theta) = \frac{|\sigma_0|}{f_\pi^2}\left[m_0|\cos(\theta/2)| + \frac{m_0 M_\pi^2}{M_{\eta'}^2}\sin^2(\theta/2)\right]. \tag{19}$$

where σ_0 is the chiral condensate at $T = \theta = 0$. Interpreting a θ dependent mass from this result, reference C is defined by

$$\begin{aligned} m_{\rm ref}(\theta) &\equiv m_{\rm C}(\theta) \\ &= m_0\cos(\theta/2) + \frac{m_0 M_\pi^2}{M_{\eta'}^2}\sin^2(\theta/2). \end{aligned} \tag{20}$$

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.

As shown in Fig. 3(b), $\tilde{M}_\pi$ in reference C slightly underestimates that of the original theory at small and intermediate θ. As shown in Fig. 3(a), however, $\langle R(\theta)\rangle$ satisfies the condition $0.5 \lesssim \langle R(\theta)\rangle \lesssim 2$ for all θ. Therefore we can think that reference C is a good reference system for any θ.

4. Summary

We have proposed a practical way of circumventing the sign problem in LQCD simulations with finite θ. This method is the reweighting method for the transformed Lagrangian (4). In the Lagrangian, the sign problem is minimized, since the P-odd mass is much smaller than the dynamical quark mass of order $\Lambda_{\rm QCD}$. 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 in the reweighting method.

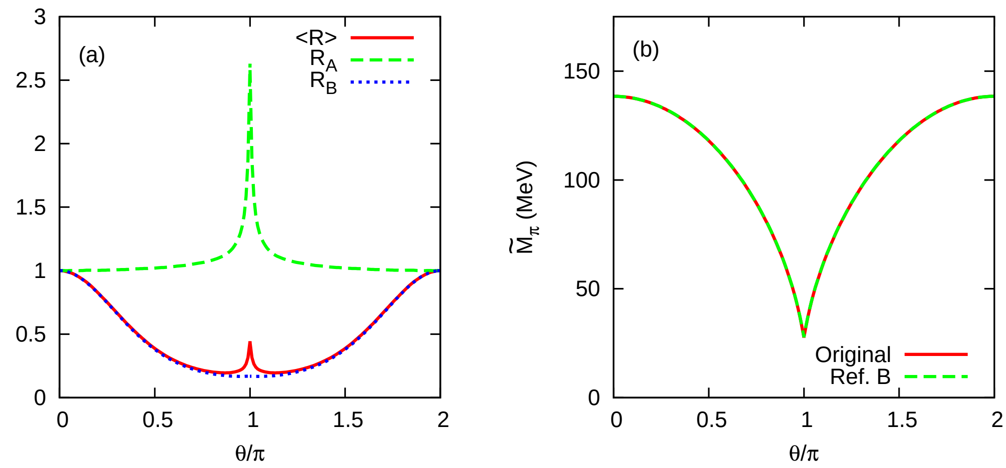

Figure 2. θ dependence of (a) the average reweighting factor and (b) $\tilde{M}_\pi$ at $T = 100$ MeV for the case of reference B.

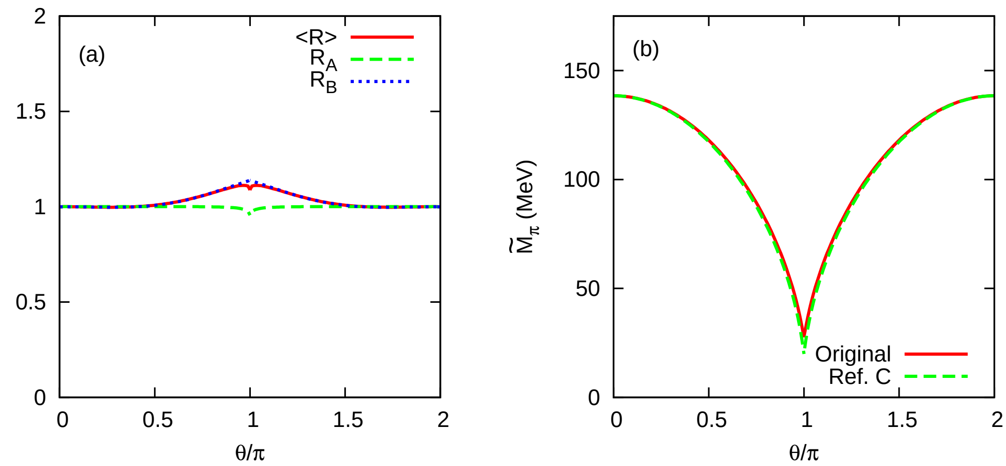

Figure 3. θ dependence of (a) the average reweighting factor and (b) $\tilde{M}_\pi$ at $T = 100$ MeV for the case of reference C.

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