Meson mass and the sign problem at finite theta

Takahiro Sasaki\textsuperscript{1}, Hiroaki Kouno\textsuperscript{2} and Masanobu Yahiro\textsuperscript{1}

\textsuperscript{1} Department of Physics, Graduate School of Sciences, Kyushu University, Fukuoka 812-8581, Japan
\textsuperscript{2} Department of Physics, Saga University, Saga 840-8502, Japan
E-mail: sasaki@email.phys.kyushu-u.ac.jp

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 $U_A(1)$ 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:

\[ \mathcal{L} = \sum_f \bar{q}_f(\gamma \partial + m_f)q_f + \frac{1}{4g^2} F_{\mu \nu}^a F_{\mu \nu}^a - i \frac{1}{64\pi^2} \varepsilon_{\mu \nu \rho \sigma} F_{\mu \nu}^a F_{\rho \sigma}^a, \]

in Euclidean spacetime. Hereafter, we will consider two-flavor QCD and assume isospin symmetry, $m_u = m_d = m_0$. Though the angle $\theta$ can take any arbitrary value theoretically, experimental measurements of neutron dipole moment give the upper limit, $|\theta| < 10^{-9}$\textsuperscript{[1, 2]}. Why should $\theta$ 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 $\theta$. After making $U_A(1)$ transformation

\[ q = e^{i\gamma_5 \frac{\theta}{2}} q', \]

$\theta$ dependence appears only through the mass term

\[ m_0(\theta) = m_0 \cos(\theta/2) + m_0 i \gamma_5 \sin(\theta/2), \]

in the transformed Lagrangian

\[ \mathcal{L} = \sum_f \bar{q}_f(\gamma \partial + m_0(\theta))q_f + \frac{1}{4g^2} F_{\mu \nu}^a F_{\mu \nu}^a. \]
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

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

$$\approx \int \mathcal{D}A \mathcal{O}' \det M_{\text{ref}}(\theta)e^{-S_g}$$

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

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

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

where $R(\theta)$ is the reweighting factor and $\det M_{\text{ref}}(\theta)$ 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 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 $\theta$, but not for large $\theta$ near $\pi$. In reference A, the limit of $\theta = \pi$ corresponds to the chiral limit for $\det M_{\text{ref}}$ that is hard for LQCD simulations to reach.

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

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

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 two-flavor NJL model in order to find out a good reference theory. We find that reference A is good only for small $\theta$, 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 $\theta$-dependent term is obtained by

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

in Euclidean spacetime where $m_0$ is the current quark mass and $\tau_0$ and $\tau_a (a = 1, 2, 3)$ are the $2 \times 2$ 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

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

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 $\langle R(\theta) \rangle$, $R_A$, and $R_B$:

$$\langle R(\theta) \rangle \approx R_A R_B,$$

$$R_A = \sqrt{\frac{\det H_{\text{ref}}}{\det H}},$$

$$R_B = e^{-\beta V(\Omega - \Omega_{\text{ref}})},$$

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

\[ H_{ij} = \frac{\partial^2 \Omega}{\partial \phi_i \partial \phi_j}, \quad \{ \phi'_i \} = \{ \sigma', \eta', \bar{a}', \bar{a}' \}, \]  

(14)

with the quark-condensates

\[ \sigma' = \langle \bar{q} q \rangle, \quad \eta' = \langle \bar{q} i \gamma_5 q \rangle, \quad \bar{a}' = \langle \bar{q} \tau q \rangle, \quad \bar{a}'' = \langle \bar{q} i \gamma_5 \tau q \rangle. \]  

(15)

The four-dimensional volume βV is obtained by βV = (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:

\[ \mathcal{L} = \bar{q} (\gamma_\mu \partial_\mu + m_{\text{ref}}(\theta)) q' - G_+ \left[ (\bar{q} q')^2 + (\bar{q} i \gamma_5 \tau q')^2 \right] - G_- \left[ (\bar{q} \tau q')^2 + (\bar{q} i \gamma_5 \tau q')^2 \right]. \]  

(16)

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

3. Numerical results

If some reference system satisfies the condition \langle R(\theta) \rangle ≈ 1, one can say that the reference system is good. As a typical example of the condition, we consider the case of 0.5 ≤ \langle R(\theta) \rangle ≤ 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

\[ m_{\text{ref}}(\theta) = m_A(\theta) = m_0 \cos(\theta/2). \]  

(17)

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

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 \text{ MeV} at \theta = 0 and 194 \text{ MeV} at \theta = \pi. As \theta increases from zero, \langle R(\theta) \rangle also increases and exceeds 2 at \theta ≈ 1.2. Reference A is thus good for \theta ≤ 1.2.

Figure 1(b) shows \theta dependence of pion mass \bar{M}_\pi at T = 100 \text{ MeV}. Since P symmetry is broken at finite \theta, P-even modes and P-odd modes are mixed with each other for each meson. Hence, \bar{M}_\pi is defined by the lowest pole mass of the inverse propagator in the isovector channel[4]. The solid (dashed) line denotes \bar{M}_\pi in the original (reference A) system. At \theta = \pi, \bar{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.

The second example is reference B defined by

\[ m_{\text{ref}}(\theta) = m_B(\theta) = m_0 \cos(\theta/2) + \frac{1}{\alpha} \left( m_0 \sin(\theta/2) \right)^2. \]  

(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 α = \bar{M}_\pi. The coefficient of the correction term is m_0^2/\bar{M}_\pi = 0.129 \text{ MeV}.

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

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

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

(19)

where $\sigma_0$ is the chiral condensate at $T = \theta = 0$. Interpreting a $\theta$ dependent mass from this result, reference C is defined by

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

(20)

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

As shown in Fig. 3(b), $\tilde{M}_\pi$ in reference C slightly underestimates that of the original theory at small and intermediate $\theta$. 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 $\theta$. Therefore we can think that reference C is a good reference system for any $\theta$.

4. 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 (4). In the Lagrangian, the sign problem is minimized, since the $P$-odd mass is much smaller than the dynamical quark mass of order $\Lambda_{QCD}$. 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. $\theta$ dependence of (a) the average reweighting factor and (b) $\tilde{M}_\pi$ at $T = 100$ MeV for the case of reference B.

Figure 3. $\theta$ 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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