QCD $\theta$-vacua from the chiral limit to the quenched limit

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Abstract

We investigate the dependence of the QCD vacuum structure on $\theta$-angle and quark mass, using the Veneziano–Di-Vecchia model. Although the Veneziano–Di-Vecchia model is a chiral effective model, it contains the topological property of the pure Yang–Mills theory. It is shown that within this model, the ground state energies for all $\theta$ are continuous functions of quark mass from the chiral limit to the quenched limit, including the first order phase transition at $\theta = \pi$ for arbitrary finite mass. Besides, based on this effective model, we discuss (i) how the ground state depends on quark mass, and (ii) why the phase transition at $\theta = \pi$ is caused both in the chiral and quenched limit. In order to analyze the relation between quark mass and $\theta$-vacua, we calculate chiral condensate as a function of quark mass. We also give a unified understanding of the phase transitions at $\theta = \pi$ in the chiral and quenched limit, making reference to the metastable states included innately in QCD $\theta$-vacuum.

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1. Introduction

An SU(N) gauge theory contains the topology which originates in non-trivial excitations of gauge field. The vacuum structure in Quantum Chromodynamics (QCD) is enormously influenced from such a topology because QCD vacuum is defined by the parameter, so-called $\theta$-angle, which enters in QCD action as the Chern–Simons term $iQ\theta$, where $Q$ denotes the winding number of gluon, $Q = \int d^4x \epsilon^{\mu\nu\rho\sigma} F_{\mu\nu}^{a} F_{\rho\sigma}^{a}$. Which $\theta$-angle is chosen in principle, therefore, is quite important for investigations of QCD phenomena. (Note that any transition between different $\theta$-vacua is forbidden in infinite volume.) The $CP^3$ symmetry in QCD, especially, depends only on the value of $\theta$-angle since the Chern–Simons term violates $CP$. The $\theta = 0$ case is the most reliable candidate maintained by an experimental result $\theta \leq 10^{-10}$ and in fact, phenomena in terms of the strong interaction seem $CP$ symmetric. Unfortunately, we do not, however, know the theoretical reason why $\theta = 0$ is selected. This is one of the unsolved problems in the standard model, referred to as the strong $CP$ problem.

One might wonder if it is necessary to study the topological property in QCD, because of the fact that $\theta$-angle takes, at most, a negligible tiny value. Nevertheless, we should consider the $\theta$-vacuum structure for investigations of QCD since there exists another origin of the topology in QCD, i.e. the axial anomaly. $\eta'$-meson, for example, acquires an extra mass much larger than the mass of other mesons, through the anomaly. With the lattice QCD simulation, it is confirmed that the $\eta'$ mass formula gives the consistent value to the observed one. We have to note here that the mass formula suggested in Ref. includes only quantities at $\theta = 0$. It is indicated, hence, that even if $\theta = 0$, the topological nature of QCD can give contributions to physics. (It is also proposed recently that dark energy could stem from $\theta$-vacuum at $\theta = 0$.)
Among many physics involved with the QCD topology, phenomena with \( \theta \neq 0 \) are on the verge of the most important subject in QCD. It has been believed that \( \theta \)-angle can be various values in event by event of heavy ion collisions [9,10]. In other words, the \( \theta \)-angle in the collision is considered as not a constant parameter but a function of the space-time coordinate (or like axion, which is the dynamical field introduced in order to solve the strong CP problem [11]). Such a new possibility of \( \theta \)-angle leads to a lot of works with respect to curious phenomena caused by the topology of QCD [12,17].

The presence of the realistic situation with a finite \( \theta \)-angle is quite suggestive for the study of \( \theta \)-vacuum. Namely, we are imposed to research what happens when \( \theta = 0 \) changes into finite values. Indeed for such a \( \theta \)-angle, the vacuum structure has already been revealed in many works through the ages, and what is important, typically, is the vacuum structure at \( \theta = \pi \) [18–37]. (See also Ref. [38], which summarizes works related to the \( \theta \)-dependence of QCD.) Naively, one might think that \( \theta = \pi \) is mere another candidate keeping QCD a CP symmetric theory, and thus \( \theta = \pi \) causes no special situation, compared with \( \theta = 0 \). Nevertheless there exists an intriguing physics at \( \theta = \pi \): the first order phase transition, i.e. spontaneous CP symmetry breaking. This is one of main points discussed in this paper.

As we have already mentioned, the axial symmetry is connected strongly with the QCD topology, as well as non-trivial gluonic excitation. We can assume, then, that the quark sector receives the topological nature belonging to the Chern–Simons. Namely, by an axial rotation of fermion field, the \( \theta \)-dependence moves to the quark mass term from the Chern–Simons term. This implies that \( \theta \)-vacua depend not only on the strong \( \theta \)-angle but also quark mass. Here, the best quantity which shows explicitly the mass-dependence of \( \theta \)-vacuum is the topological susceptibility interpreted as a function of quark mass, \( \chi_{\text{top}}(m) \). Indeed the topological susceptibilities in the chiral limit and the quenched limit have quite different forms as a function of the mass. It is obvious, hence, that we should investigate the mass-dependence of \( \theta \)-vacuum, in order to understand completely the topological nature in QCD. Nevertheless, the vacuum structure for arbitrary quark mass has not been studied in detail except for the chiral theory and the pure gluonic theory. (See Ref. [39], where comparing the cases that \( N_f = 0 \) and that \( N_f \neq 0 \), differences between the chiral and quenched limit are argued.) Briefly speaking, we do not know the vacuum structure for quark heavier than \( \Lambda_{\text{QCD}} \), and no effective theory including \( \theta \)-angle is known. (In Ref. [40], for example, it is pointed out that effects of the axial anomaly exist definitely in the heavy quark effective theory, but how to calculate these contributions to dynamics is not found.)

The Veneziano–Di-Vecchia model [41] is one of the simplest, but remarkable chiral effective models reflecting topological properties of QCD, and thus dynamics described by this model have been investigated from many aspects [2,10,42,44]. (Additionally, since the inhomogeneous \( \theta \) can be regarded as the dynamical \( \eta' \) field, it is possible to discuss the phenomena related to \( \theta \) and electromagnetic field \( B \), based on the Veneziano–Di-Vecchia model [45].) In this paper, we discuss the \( \theta \)-vacuum structure from the point of view of the mass-dependence, within the Veneziano–Di-Vecchia model. We mention the relation between quark mass and the topology more specifically in Sec. 2. In order to reveal the effect of quark mass for \( \theta \)-vacuum, we calculate the vacuum energy for arbitrary quark mass in Sec. 3. This result obtained from the Veneziano–Di-Vecchia model is supported in Sec. 4 by the enforcement that this model is not a mere chiral model with the QCD topology, but a more remarkable model, which includes even the feature of the axial anomaly and \( \theta \)-vacua in the quenched limit. In other words, the suggestion from this chiral model is quite pedagogical even for large mass compared with \( \Lambda_{\text{QCD}} \). By calculating chiral condensate as a function of quark mass with this model, we can see in Sec. 5 the dynamical mechanism of \( \theta \)-vacuum, specifically the role of quark mass for the decision of vacuum states. Moreover, we investigate the first order phase transition at \( \theta = \pi \), which is quite beneficial physics for the understanding of the vacuum structure as a function of quark mass. It is important, here, that the phase transition in the chiral limit and the one in the quenched limit seem naively similar although the dynamics in two limits are completely different. In Sec. 6 we discuss the origin of such a similarity of the vacuum structure, on the basis of the degeneracy of the metastable vacua included in QCD vacuum.

2. Mass-dependence of \( \theta \)-vacuum

Quark mass is one of the most important factors in the discussion of the topological property of QCD. Let us review the global symmetries in QCD and the axial anomaly here, in order to find the mass-dependence of \( \theta \)-vacuum. Classical Lagrangian of massless QCD with \( N_f \) flavors is invariant under a transformation related to the global symmetry group \( \text{SU}(N_f)_L \times \text{SU}(N_f)_R \times \text{U}(1)_Y \times \text{U}(1)_A \). By contrast, in quantum theory, there dose not exist the axial
symmetry $U(1)_A$ due to the axial anomaly. As a result, the measure of the functional integration for the quark field changes under the $U(1)_A$-rotation with a phase $\alpha$ as $Dq \to Dq \exp(-iN_\alpha \omega)$, where $\omega$ denotes the winding number density i.e., $\int d^4x \omega = Q$. The measure for anti-quark field is transformed similarly. Thus by the rotation, the extra term is added to the Lagrangian; $\mathcal{L} \to \mathcal{L} - 2N_\alpha \omega$. Choosing the rotation angle as $\alpha = \theta/2N$, one can then vanish the Chern–Simons term $iQ\theta$. In massive QCD, however, $\theta$-angle remains still in Lagrangian even though one takes such a rotation angle, due to an extra factor added to the quark mass term, which is not invariant under the $U(1)_A$ rotation; $m \to me^{\gamma\theta/2N}$. Hence one can write schematically the transformation of QCD action, as follows:

$$S_\theta = S(m) + i\theta \to S_\theta = S(m e^{\gamma\theta/2N}).$$

(1)

This means that there appears the $\theta$-dependence of QCD only through quark mass, and thus the $\theta$-vacuum structure depends not only on $\theta$ but also on $m$.

The mass-dependence of QCD $\theta$-vacua emerges in typical limits; the chiral limit and the quenched limit. In these two limits, the topological susceptibility

$$\chi_{\text{top}} = \frac{1}{V_4} \int d^4x \omega(x)\omega(0) \big|_{i\omega=0},$$

(2)

for example, takes completely different values. The lattice QCD simulation shows that the susceptibility in the pure Yang–Mills theory is a constant; $\chi_{\text{top}} = \chi_{\text{pure}} \sim (170 - 180\text{MeV})^4$ [46]. On the other hand, it is derived that for small quark mass, the topological susceptibility is proportional to the mass; $\chi_{\text{top}} \propto m$ [23]. (This is consistent to that the $\theta$-dependence through the mass term is vanished in the chiral limit, as shown in Eq. (1).) Since the topological susceptibility is the potential curvature of $\theta$-vacuum at $\theta = 0$, the difference of the topological susceptibilities in two limits indicates actually that the vacuum structure depends on quark mass.

For middle mass i.e., finite large mass, the $\theta$-vacuum structure is, however, not clear. This is because neither a heavy quark effective model or theory including $\theta$-angle is not known, and thus there is no method to calculate the physical quantities under the presence of $\theta$-angle, for heavy quarks compared with $\Lambda_{QCD}$, i.e., $c$, $t$, and $b$-quarks. The unclarity of the $\theta$-vacuum for large mass might be realized if one reconsiders the $\theta$-vacuum in the pure Yang Mills theory, comparing with the one in the heavy quark theory. In general, degree of freedom in theory is dynamical field. Heavy quark does not, therefore, engaged in dynamics, or the propagations for heavy flavors become negligible as the masses increased. This can be rephrased in terms of field theory as follows; the pure Yang–Mills theory is regarded as the theory after one integrate out heavy flavors. From a naive calculation, however, this procedure to obtain the pure Yang–Mills theory from QCD would lead to a wrong $\theta$-dependence. By the $U(1)_A$-rotation, $q \to e^{\gamma \theta/2N} q$, as have already mentioned, the Chern–Simons term is vanished, and instead of this, the $\theta$-angle appears only in the mass term. If starting from this axial rotated action, hence, one could integrate out heavy quark, then $\theta$-angle also have been removed from the action. This result that there would exist no $\theta$-dependence in the pure Yang–Mills theory is quite weird since one can obtain the pure Yang–Mills theory with the definite $\theta$-dependence, starting from the action before the rotation. In fact, the topological susceptibility in the pure Yang–Mills theory is a finite value $\chi_{\text{pure}}$, as mentioned.

This wrong result might be caused due to the non-commutativity of taking the large mass limit and the regularization of the axial anomaly (and indeed, we see the cause of the non-commutativity for the vacuum state in a later section). This implies, however, that the heavy quark approximation with $\theta$-angle is never trivial and the pure Yang–Mills theory does not derived straightforwardly from full QCD. Therefore, we should take care the quenched theory under the presence of $\theta$-angle. Additionally the non-commutativity imposes us to analyze more particularly the $\theta$-vacuum structure depending on quark mass. Namely, it is necessary to investigate the dynamical effect of quark mass to the $\theta$-vacuum state. We discuss such an effect of quark mass in Sec.5 by the estimation of the chiral condensate as a function of quark mass.

The physics at $\theta = \pi$ is one of the most intriguing points in the investigation for $\theta$-vacua, and also a good example that demonstrates the mass-dependence of $\theta$-vacua. As mentioned in Sec.1 $\theta = \pi$ is related to the important feature of $\theta$-vacuum; the first order phase transition [18]. Using, the Veneziano–Di-Vecchia model, which is a chiral effective model involving the $U(1)_A$ anomaly in full QCD, one can see that the phase transition happens at $\theta = \pi$ [20]. It is suggested that also in the quenched theory, i.e., the pure Yang–Mills theory, the first order phase transition occurs, by the investigations with the holographic approach [31]. These phase transitions, one in the chiral theory and the other in the pure Yang–Mills theory, might seem an inherent feature involving in $\theta$-vacuum. We should note, however, that
this similarity is never trivial, and indeed these phase transitions come from completely different causes. The phase transition at $\theta = \pi$ in the chiral effective model results from the dynamics of meson fields or quarks. On the other hand, in the pure Yang–Mills theory, of course, there are only gluons as the trigger for the transition. Additionally, the formations of the metastable states which leads to the phase transitions are definitely different in the chiral and quenched limit. While in the quenched limit, there are infinite non-degenerate metastable states, the metastable states in the chiral limit are categorized into only few patterns. This difference with respect to the metastable states implies, hence, that the degeneracy originates in the number of dynamical flavors. We discuss in Sec. 5 including the point of view of the relation between dynamical flavors and metastable states, the difference of the first order phase transitions in the chiral and quenched limit, based on a common framework.

3. Veneziano–Di-Vecchia model

Let us discuss the $\theta$-dependence of QCD with quark mass regarded as a parameter, using the Veneziano–Di-Vecchia model [41], which is described as the following Lagrangian,

$$\mathcal{L}_V = \frac{f_\pi^2}{4} \text{tr}[(\partial_\mu U^\dagger \partial^\mu U + 2\chi(MU^\dagger + UM)] - \frac{X_{\text{pure}}}{2} \left[\theta - \frac{i}{2} \text{tr}(\ln U - \ln U^\dagger)\right]^2,$$

where $f_\pi$ is the pion decay constant and $\chi = -(q\bar{q})/f_\pi^2$ is a parameter given by the Gell-Mann-Oakes-Renner relation. First we extend the argument in Ref. [20] to the case for arbitrary quark mass. (The validity of the extension will be discussed in Sec. 4). We consider two quarks with a degenerate mass, i.e., $M = \text{diag} (m, m)$. Since we are interested in the ground state energy, the dynamical field is set as $U = \text{diag} (e^{i\phi_u}, e^{i\phi_d})$. The potential part of Eq. (3) can then be reduced to a simpler form;

$$V(\phi_u, \phi_d) = -f_\pi^2 \chi_m \cos(\phi_u + \phi_d) + \frac{X_{\text{pure}}}{2} (\theta + \phi_u + \phi_d)^2.$$  

In order to find the QCD vacuum, we have to solve the following equation of motion

$$f_\pi^2 \chi_m \sin \phi_i + X_{\text{pure}} (\theta + \phi_u + \phi_d) = 0, \quad i = u, d,$$

which implies $\sin \phi_u = \sin \phi_d$. There are then two solutions for Eq. (5): $\phi_u = \phi_d + 2\pi k = \phi$ and $\phi_u = (2k - 1)\pi - \phi_d = \phi$. The potentials Eq. (4) for the latter types are not negative and independent on $\phi$. On the other hand, as we see in the numerical result, the former types always give zero or negative potentials, and thus they can be the solutions. Inserting the solution for $k = 0$, i.e. $\phi_u = \phi_d = \phi$ into Eq. (5), we obtain the simplest equation,

$$f_\pi^2 \chi_m \sin \phi + X_{\text{pure}} (\theta + 2\phi) = 0.$$  

It is straightforward to find the energy $V(\phi, \phi)$ only in the chiral and quenched limit, although we cannot solve the transcendental equation analytically. The solutions read

$$\phi(\theta, m) = \begin{cases} -\frac{\theta}{2} + O(m) & \text{(small } m) \\ \frac{\theta X_{\text{pure}}}{f_\pi^2 \chi m} + O(m^{-2}) & \text{(large } m) \end{cases}$$

which give the minimum potential energy for small and large quark mass represented as

$$V(\phi, \phi) = \begin{cases} -2f_\pi^2 \chi_m \cos \frac{\theta}{2} + O(m^2) & \text{(small } m) \\ -2f_\pi^2 \chi_m + \frac{X_{\text{pure}}}{2} \theta^2 + O(m^{-1}) & \text{(large } m) \end{cases}.$$  

Note that the $\theta$-dependences of the minimum potential in the two limits are decided by the amplitude of quark mass, compared with the dimensional quantity $X_{\text{pure}}/f_\pi^2 \chi$; the potential becomes sinusoidal or parabolic for small or large
mass, respectively. (We shall mention the detail of the contribution from the quark mass at the end of this section.) Also the numerical result of the potential energy for arbitrary quark mass is shown in Fig. 1. Here we substituted $V_{\text{pure}} = (170 \text{ MeV})^4$.

The potential in Fig. 1 is clearly not the true $\theta$-vacua since the periodicity of $\theta$ is not 2$\pi$ but 4$\pi$. Now we consider the general solutions for Eq. (5), $\phi_u = \phi_d - 2\pi k = \phi$, and then solve the equation,

$$f^2 \chi m \sin \phi + \chi_{\text{pure}} (\theta + 2\pi k + 2\phi) = 0.$$  

Because this can appear as the equation where $\theta$ in Eq. (6) is shifted by $2\pi k$, it is found simply that the potential energy for this solution $\phi_u = \phi_d - 2\pi k = \phi$ is the following form;

$$V(\phi, \phi + 2\pi k) = \begin{cases} -2f^2 \chi m \cos \left(\frac{\theta + 2\pi k}{2}\right) + O(m^2) & \text{(small m)} \\ -2f^2 \chi m + \frac{\chi_{\text{pure}}}{2}(\theta + 2\pi k)^2 + O(m^{-1}) & \text{(large m)} \end{cases}$$

In the small mass limit, all potentials for odd $k$ are identical to $V(\phi, \phi + 2\pi)$ and less than $V(\phi, \phi)$ at $\pi \leq \theta \leq 3\pi$, $5\pi \leq \theta \leq 7\pi$ and so on while $V(\phi, \phi + 2\pi k)$ for even $k$ are equal to $V(\phi, \phi)$. As mentioned in Ref. [20], hence for small mass the minimum potential is decided by the competition of two infinitely degenerate ground states with even $k$ and odd $k$. On the other hand, we also obtain the property of the pure Yang–Mills theory from the investigation of the Veneziano–Di-Vecchia model in the large mass limit. The minimum energy for large mass is given by combining all different parabolic functions $\sim (\theta + 2\pi k)^2$, which is consistent to the one derived from the pure Yang–Mills theory [31]. Additionally, as shown in Fig. 2 the minimum potential calculated with this effective model declares that continuity of $\theta$-vacua, including the first order phase transitions at $\theta = (2n - 1)\pi$ for arbitrary integer $n$.

We understand why the vacuum energies for small and large mass are described as different functions of $\theta$-angle, considering from the structure of Eq. (6) and the solution Eq. (7) again. As mass increased, the solution $\phi(\theta, m)$ Eq. (6) becomes smaller, and eventually approaches to zero, as described in Eq. (7). In other words, quark mass plays the role to fix the dynamical meson field $U$ to unity. This gives the explanation for the question raised in Sec. 1 i.e., the reason why in the pure Yang–Mills theory with the Chern–Simons term $iQ\theta$ cannot be vanished by the $U(1)_{\Lambda}$ rotation, unlike in light flavor QCD, as follows. In this effective model a $U(1)_{\Lambda}$ rotation adds a phase factor to the chiral field $U$, and thus the phase of $U$ is shifted by the rotation. Then if quark is enough heavy, the axial rotation leaves up the state at the bottom of the potential valley i.e., $U = 1$. For large mass, hence, the $U(1)_{\Lambda}$-transformation is prohibited energetically.
4. Topological susceptibility

Although using the Veneziano–Di-Vecchia model, we obtained the landscape of the ground state energy as a function of quark masses and θ-angle, one might wonder why the low-energy model can give such a continuous structure even for large mass. In order to confirm the validity of the above discussion with respect to QCD θ-vacua by using the Veneziano–Di-Vecchia model for arbitrary quark mass, we calculate the topological susceptibility within this model. Since the topological susceptibility is the potential curvature at \( \chi_{\text{top}} \) for Eq. (6). Thus the we find the topological susceptibility as a function of quark mass [43]:

\[
\chi_{\text{top}}(m) = \frac{\partial^2 V}{\partial \theta^2} \bigg|_{\theta=0} = \left[ \frac{\partial^2 \phi}{\partial \theta^2} \frac{\partial V}{\partial \phi} + \left( \frac{\partial \phi}{\partial \theta} \right)^2 \frac{\partial^2 V}{\partial \phi^2} \right]_{\theta=0.}
\]

The mass-dependence of the topological susceptibility is indicated in Fig. 3. This function shows not only that the topological susceptibility in the chiral limit is a linear function of quark mass but also that the one in the large mass limit approaches to the constant value \( \chi_{\text{pure}} \). Eq. (11) implies, hence, that the Veneziano–Di-Vecchia model contains the information of the topology not only in the chiral limit but also in the quenched limit.

It is not accidental that the Veneziano–Di-Vecchia model includes even the topological property in the large mass limit. The topology in this model is introduced under the U(1) symmetry. As well-known, the chiral condensate with a finite η-angle becomes a complex value, because under the U(1) symmetry, there is no dynamical quark after one performs integrating out all flavors. This situation is equivalent to the one in the large mass limit. The topological property in the pure Yang–Mills theory, therefore, enters automatically in the Veneziano–Di-Vecchia model.

Higher order mass terms is neglected in our discussion with the Veneziano–Di-Vecchia model, and thus in order to find the exact vacuum structure for large mass, we should include all the correction terms of quark mass. Nevertheless, the topological susceptibility Eq. (11) and the vacuum energy function of θ-angle Eq. (10) shows that the θ-vacuum state calculated with the Veneziano–Di-Vecchia model in the large mass limit becomes exactly the expected form in the pure Yang–Mills theory, in spite of the calculation without any higher corrections. The Veneziano–Di-Vecchia model can, therefore, be regard as the simplest model which satisfies two boundary conditions, i.e. the topological property in the chiral limit and the quenched limit. Then we emphasize that the Veneziano–Di-Vecchia model is quite pedagogical for the investigation of the θ-vacuum structure dependent on quark mass, and at least, the vacuum states for enough small and large mass can be obtained correctly from this effective model.

5. Chirality

By evaluating chiral condensate as a function of quark mass and θ-angle, we see again the contribution of mass to θ-vacua, and give the new suggestion for the hadron condensate with the θ-dependence. As well-known, the chiral condensate with a finite θ-angle becomes a complex value, because under the U(1)_A-rotation with the angle \( \theta/2N_f \), the mass term is transformed as

\[
m\bar{q}q \rightarrow m\bar{q}e^{i\pi\theta/N_f}q
\]

\[
= m\bar{q}q \cos(\theta/N_f) + im\bar{q}y\bar{q}q \sin(\theta/N_f).
\]

Since we regard the chiral condensate as \( m\bar{q}q \) with phases \( \phi_q \) and \( \phi_d \) in our argument, its real part (or ρ-condensate) and imaginary part (or η-condensate) can be obtained directly from the solution \( \phi(\theta, m) \) for the minimized equation Eq. (5):

\[
\text{Re}\langle\bar{q}q\rangle_{\theta} = \langle\bar{q}q\rangle \cos \phi(\theta, m), \quad \text{Im}\langle\bar{q}q\rangle_{\theta} = \langle\bar{q}q\rangle \sin \phi(\theta, m).
\]

where \( \langle\bar{q}q\rangle \) stands for the chiral condensate for \( \theta = 0 \). (One can confirm from the solution Eq. (5), the consistency of the condensates Eq. (13) to that the complex chiral condensate becomes the real chiral condensate \( \langle\bar{q}q\rangle \) for \( \theta = 0 \).) The mass- and θ-dependences of the condensates are shown in Fig. 4.
Figure 3. The topological susceptibility as a function of quark mass. For small mass the topological susceptibility is a linear function of quark mass. On the other hand for large mass the topological susceptibility is asymptotically equal to $\chi_{\text{pure}}$. The two green lines denote $\chi_{\text{top}}(m) = mf^2_\pi \chi/2$ and $\chi_{\text{top}}(m) = \chi_{\text{pure}}$, respectively. The Veneziano–Di-Vecchia model, therefore, include the vacuum structure both in the chiral and quenched limit.

Figure 4. $\theta$- and mass-dependence of the complex chiral condensate. For both condensates, there are singularities at $\theta = \pi$. (The same result is pointed out for small mass in Ref. [33].) These condensates for large mass do not depend on $\theta$-angle, and especially the imaginary part is suppressed. This is becaus the phase of meson field $U$, i.e. $\phi_{ud}$ are fixed dynamically to zero for heavy quark mass. Therefore, the chiral condensate for large mass is also fixed to the real direction in the chiral circle.

We have to give, here, some remarks in terms of the chiral condensate as a function of quark mass. As discussed in Sec. [3] the solution for large mass is fixed to zero. As a result of this, the imaginary part of the complex chiral condensate $\sim \sin \phi$ decreases as quark mass increased (see the right panel of Fig. [4]). This means that the complex chiral condensate, even for finite $\theta$-angle, becomes a real value in the large mass limit. In other words, as well as $\phi$ is fixed to zero by large mass, the complex chiral condensate is also fixed to real direction on the chiral circle, due to the effect of large mass. Besides, based on such a fixation mechanism of chiral condensate, we can obtain an answer for the question given in Sec. [2] i.e., why taking the quenched limit after the axial rotation Eq. (12) leads to a weird action without the topology. Namely, the real direction of the chiral condensate on the complex plane is most favorable and thus the axial rotation in the large mass limit cannot be performed energetically.

For light quark, we find also typical behaviors in Fig. [4]. As long as quarks are quite light, the $\theta$-dependence of the imaginary part remains because there is no energetic restriction of the axial rotation. Moreover, the discontinuities in Fig. [4] come from the one of the potential Fig. [3]. Indeed it is pointed out that in the chiral theory, the condensates have such a remarkable singularity at $\theta = \pi$ (see also Ref. [29] as the similar discussion of the massive Schwinger model).
6. Metastable states

In this section, we discuss metastable states, which is the origin of the first order phase transitions at \( \theta = \pi \), included in QCD vacuum. In order to do this, first we review a remarkable work in which the nature of the metastable state is discussed in Ref. [47], as follows.

The QCD partition function with \( \theta \)-angle is given by the following form,

\[
Z(\theta) = \sum_{Q} Z_{Q} e^{i\theta Q} = \sum_{Q} f(Q) e^{i\theta V_{4}Q}.
\]  

(14)

Here, we introduced the topological charge density \( \tilde{Q} = Q/V_{4} \), where \( V_{4} \) denotes the four dimensional volume. (Note that we used and will use different notations from the one in the original paper Ref. [47], e.g., the definition of the partition function for the topological sector \( \tilde{Q} \) in Eq. (14), the normalization in Eq. (15), and so on.) From this partition function, taking the large volume limit i.e., the continuous limit \( \tilde{Q} \to x \), its continuous version is obtained;

\[
Z(\theta) \to Z_{c}(\theta) = V_{4} \int dx f(x) e^{i\theta V_{4}x}.
\]  

(15)

Then using the Poisson summation formula [47], one can obtain the relation between these two partitions \( Z(\theta) \) and \( Z_{c}(\theta) \) as

\[
Z(\theta) = \sum_{k} Z_{c}(\theta + 2\pi k).
\]  

(16)

This relation implies that there exist infinite metastable vacuum states because the partition function \( Z(\theta) \) receives the dominant contribution from only one metastable state sector in the large volume limit. Namely, the energy density of QCD becomes the one in the dominant sector;

\[
-\frac{1}{V_{4}} \ln Z(\theta) \to \min_{k} \left[ -\frac{1}{V_{4}} \ln Z_{c}(\theta + 2\pi k) \right].
\]  

(17)

We have to note that as pointed out in Ref. [47], an integer \( k \) is nothing to do with the label related to topological sectors, i.e. \( Q \) or \( x \). Indeed the partition function in respect to a \( k \)-th metastable state includes the contributions from all topological sectors (see Eq. (15)).

In this context, let us see \( CP \) symmetry. Due to the summation in Eq. (16), the topological charge density is also given by the sum of the contributions from all sectors;

\[
\langle \tilde{Q} \rangle = \sum_{k} \langle x \rangle_{k}, \quad \langle x \rangle_{k} = \frac{V_{4}}{Z(\theta)} \int dx f(x) e^{i(\theta + 2\pi k) V_{4}x}.
\]  

(18)

One can confirm that \( \langle \tilde{Q} \rangle \) vanishes at \( \theta = \pi \) because of the cancellation between all adjacent pairs, e.g., \( \langle x \rangle_{0,0,=\pi} = -\langle x \rangle_{-1,0,=\pi} \), and thus there is \( CP \) symmetry at \( \theta = \pi \). In the large volume limit, however, \( CP \) might be broken. This is because for large volume, only one dominant metastable sector remains in the summation Eq. (16) and so in Eq. (18).

It is possible, hence, that the total topological charge density \( \langle \tilde{Q} \rangle \) becomes finite, as long as the density in the dominant sector is not zero.

From this argument, the spontaneous \( CP \) breaking is understood as follows. In the large volume limit, the 0-th sector is dominant at least for the small \( \theta \) (see Eq. (15)). Additionally, suppose a typical case that the 0-th sector is dominant even for \( 0 \leq \theta \leq \pi \), then so is the −1-th sector for \( \pi \leq \theta \leq 3\pi \). We drew each domains in the upper part of Fig. 5 and the one of Fig. 6. Therefore, there is the first phase transition at \( \theta = \pi \) if the charge density does not vanish at \( \theta = \pi \). (If not, i.e., \( \langle x \rangle_{0,0,=\pi} = 0 \), then there is not a phase transition but a crossover at \( \theta = \pi \) since \( \langle x \rangle_{-1,0,=\pi} = -\langle x \rangle_{0,0,=\pi} = 0 \).) Note that although a few assumption is necessary in the above discussion, we arrived at the phase transition without a typical model. In this sense, this is the general mechanism of the first order phase transition at \( \theta = \pi \) [47].

Then we investigate the phase transition at \( \theta = \pi \) from the point of the relation between quark mass and the metastable state. In the pure gluonic theory, the energy density of \( \theta \)-vacuum is given by [31],

\[
E(\theta) \propto \min_{k} (\theta + 2\pi k)^{2}.
\]  

(19)
This energy configuration shows the one-to-one correspondence between the integer $k$ in Eq. (19) and the label of the metastable states in Eq. (16) (see Fig. 5). All metastable states suggested in Ref. [47], therefore, are not degenerate if there is no dynamical quark. On the other hand, for small masses there are only a few types of the vacuum states [20]. These a few states can, hence, be interpreted as the infinitely degenerate states made up by the infinite metastable states discussed in Ref. [47] (see Fig. 6). Indeed Eq. (10) shows that the potential energies for small mass are separated by the two types corresponding to an odd $k$ and an even $k$. In other words, the vacuum energy for the two light flavors case is given by

$$E(\theta) \propto \min_{k=2n,2n-1} \cos \left( \frac{\theta + 2\pi k}{2} \right).$$

(20)

These differences of the degeneracies in the chiral and quenched limit is understood uniformly with the Veneziano-Di Vencchia model. Let us consider again the $N_f$ flavors potential given by

$$V(\phi_f) = -f_s^2\chi m \sum_f \cos \phi_f + \frac{\chi_{\text{pure}}}{2} \left( \theta + \sum_f \phi_f \right)^2,$$

(21)

which leads to the set of the equations

$$f_s^2\chi m \sin \phi_f + \chi_{\text{pure}} \left( \theta + \sum_f \phi_f \right) = 0,$$

(22)

where $k_f$ is an integer and $f = 1, \cdots, N_f$ denotes the label of flavors. Since we have the equation of motions $\sin \phi_f = \sin \phi_{f'}$ for any $f$ and $f'$, the general solution which minimizes the potential takes the form as

$$\phi_f = \phi + 2\pi k_f.$$

(23)

(Note that other type solutions, such as $\phi_1 = \pi - \phi_2$ do not give the minimum, as mentioned in Sec. 3.) The true solution for enough heavy quarks is, however, given by $\phi = 0$ because the mass terms $-\cos(\phi + 2\pi k_f)$ should
become much smaller. We, hence, find the potential for large mass as
\[
V = -N_f f_\pi^2 \chi m + \frac{\chi_{\text{pure}}}{2} (\theta + 2\pi k)^2,
\]
where \(k\) was defined as the sum of \(k_f\). Therefore, subtracting the mass term from this ground state energy for heavy quarks, we obtain the one of the pure Yang–Mills theory, i.e. the parabolic type potential (19). (In the pure Yang-Mills theory, there is, of course, no mass term.)

Let us consider the case for small mass. Then the topological term \(\sim (\theta + \phi_1 + \phi_2 + \cdots)^2\) should be almost zero as well as the mass terms in the small mass limit. Hence, the solution for the case with \(N_f\) degenerate light flavors approximately satisfies the following simple equation of motion,
\[
\theta + \sum_f \phi_f = 0,
\]
and thus, \(\phi\) is given by
\[
\phi = -\frac{\theta + 2\pi k}{N_f},
\]
where \(k\) was defined as the sum of \(k_f\). This condition for \(\phi\) implies that there exist the \(N_f\) independent solutions. (The replacement \(k = 1 \to k = N_f + 1\) means \(k_f \to k_f + 1\) for all \(f\).) Then, by inserting the solution Eq. (23) with \(\phi\) given by Eq. (26) into the potential Eq. (21), we obtain
\[
V = -N_f f_\pi^2 \chi m \cos \left(\frac{\theta + 2\pi k}{N_f}\right),
\]
which shows that there are \(N_f\) energy configurations corresponding respectively the \(N_f\) solutions deciding the true vacuum, as well as the vacuum in \(N_f = 2\) flavor theory consists of the two cosine functions in Fig. 6. The infinite metastable states defined by Eq. (19), therefore, degenerate into \(N_f\) states, due to the existence of \(N_f\) dynamical flavors.

Considering the dynamics of heavy quarks, one can find more clearly the relation between the degeneracy of the metastable states and the number of flavors. For example, suppose that there are one heavy flavor named \(\phi_1\), and two light flavors, \(\phi_2\) and \(\phi_3\). As well as the phases of light flavors are decided so that the topological term is much smaller, the heavy flavor \(\phi_1\) is fixed to zero because the mass term for heavy flavor has to be small, as discussed also in Sec. 5. This situation is, therefore, equivalent to the case that there are only two dynamical flavors as shown in Fig. 7 and thus the degeneracy of the metastable states is equal to not the number of the flavors included originally in theory, but the one of dynamical quarks.

As an application of the above discussion, we can lead to an interesting result for one flavor case, from the Veneziano–Di-Vecchia model. Based on the degeneracy of the metastable states, there is no phase transition for the one light flavor case, due to adjacent regions are dominated by only one sector. On the other hand, the potential in the large mass limit is given by Eq. (19) independently on \(N_f\), and thus there appears the phase transition at \(\theta = \pi\). This implies that, therefore, for \(N_f = 1\), there is a phase transition (strictly speaking, a crossover) in terms of the absence and existence of the phase transition at \(\theta = \pi\). Then we can actually confirm such a transition from the solution for the one flavor case \(\phi_1 = \phi\), which is the order parameter of the phase transition. (Here we can neglect \(2\pi k_1\) because there is only one solution for \(N_f = 1\).) In Fig. 8 the first order phase transition appears for \(m \gtrsim f_\pi\), while the solution is a smooth function of \(\theta\)-angle. The same result as this was argued in Ref. [25, 26].

7. Conclusion

We showed in this paper how quark mass configurations to QCD \(\theta\) vacua with the Veneziano–Di-Vecchia model, considering the mass and the strong \(\theta\)-angle as parameters. The discussions in this paper are on the basis of a new interpretation for the model, i.e. the possibility to suggest the physics even for the case that quarks possess large mass. First of all, we investigated the effect of heavy quark to the \(\theta\) vacuum state, calculating the potential energy in the Veneziano–Di-Vecchia model. Then we derived the fact that for large mass, the solution, i.e., the phase of meson field minimizing the potential is fixed to zero. This gives an answer for a naive question; why taking the large mass limit
and the axial rotation cannot be commutative. Namely, such a solution for large mass indicates that any axial rotation for large mass is forbidden energetically since the rotation cannot change the phases of meson field stuck to zero in the large mass limit. We also confirmed that this argument is valid, from the calculation of chiral condensate for arbitrary quark mass. For large mass, the complex chiral condensate after the axial rotation i.e., $(\bar{q} q)^{\psi(\hat{\theta})/N_f}$ is fixed to the real value because the condensate in the Veneziano–Di-Vecchia model is also decided by the phase of the meson field.

We obtained the \(\theta\)-vacuum structure as a function of quark mass. As pointed out in Ref. [47], QCD \(\theta\)-vacuum includes concommitantly infinite many metastable states which are different from the topological vacua labeled by the Chern–Simons number. In the quenched limit, the vacuum energy is given by the one of the infinite non-degenerate metastable states [31]. In contrast, there are only \(N_f\) metastable states for the chiral effective model [20]. Such a difference implies that dynamical quarks play role to lead to the degeneracy of the metastable states underlying in full QCD. In fact, this is shown with the Veneziano–Di-Vecchia model; while infinitely many metastable states are completely non-degenerate for the case that there is no dynamical quark, there are \(N_f\) degenerate metastable states for the dynamical \(N_f\) flavors case. Our calculation exhibits, additionally, that the \(\theta\)-vacuum structure in the shape of the cosine curves is transformed into the parabolic configuration, with increasing quark mass. Nevertheless, the structure at the \(\theta = \pi\) does not change. Namely, there are first order phase transitions at \(\theta = \pi\) for arbitrary finite quark mass.

Based on the Veneziano–Di-Vecchia model, the phase transitions for arbitrary finite mass is interpreted uniformly as follows. In general, if the critical \(\theta\)-angle at which a dominant metastable sector changes into a different one is equal to \(\pi\), only one metastable sector is, independently on quark mass, selected as the dominant one in each range \((2n-1)\pi \leq \theta \leq (2n+1)\pi\) [47]. Since in the pure Yang–Mills theory, all dominant sectors have different, i.e. completely non-degenerate parabolic energy configurations, it is clear that the phase transition happens at \(\theta = \pi\) in this limit. To the contrary, the vacuum energy of all dominant sectors for small mass are categorized into only a few
cosine curves, and thus they are infinitely degenerate. In this case, it is not always true that there is also such a phase transition in the chiral model. If adjacent regions, e.g. $-\pi \leq \theta \leq \pi$ and $-3\pi \leq \theta \leq -\pi$, were dominated by a same metastable sector, then there would be no phase transition at the boundary between these two. The metastable states for small mass derived from the Veneziano-Di Vecchia model are, however, given by cosine curves, and the dominant sectors of adjacent regions are always different. As a result of this, there are phase transitions for arbitrary finite mass. (Note that the transition in the one light flavor model does not happen since there is only one metastable state.) The similarity of the phase transitions in the two different theories, i.e. the chiral and quenched theory, hence, results from the existence of similar, but different formations of metastable states, which are created by $N_f$ degenerate states, and infinite non-degenerate states in the small and large mass limit, respectively.

Finally, we stress that one should investigate more the property of $\theta$-vacua, especially in regard to the mass-dependence. For example, we need to discuss the heavy quark effective theory, considering the $\theta$-vacuum. Such an approach might give supports for our calculation based on Veneziano–Di-Vecchia model. At the same time, the numerical simulation instead of Lattice QCD, which does not work for finite $\theta$-angle, also has to be performed for the $\theta$-vacuum structure [48, 49]. Besides, combining this new effective theory with the locally $P$ and/or $CP$ violating domains in the collision [40, 48], the discussion of the $\theta$-dependence for large mass would be quite fruitful for the heavy flavors, which are the important probes in order to identify the initial state of the relativistic heavy ion collision. Conversely, from a new actual estimation of the energy loss of the heavy quark jet [50, 51] with consideration of $\theta$-vacuum for large mass, one could obtain the information of the locally $P$ and/or $CP$ violating bubbles in the collision.

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