Pion Masses in Two-Flavor QCD with η Condensation

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We investigate some aspects of two-flavor QCD with $m_u \neq m_d$ at low energy, using the leading order chiral perturbation theory including anomaly effects. While nothing special happens at $m_u = 0$ for the fixed $m_d \neq 0$, the neutral pion mass becomes zero at two critical values of m_u, between which the neutral pion field condenses, leading to a spontaneously CP broken phase, the so-called Dashen phase. We also show that the "topological susceptibility" in the chiral perturbation theory diverges at these two critical points. We briefly discuss a possibility that $m_u = 0$ can be defined by the vanishing the "topological susceptibility. We finally analyze the case of $m_u = m_d = m$ with $\theta = \pi$, which is equivalent to $m_u = -m_d = -m$ with $\theta = 0$ by the chiral rotation. In this case, the η condensation occurs at small m, violating the CP symmetry spontaneously. Deep in the η condensation phase, three pions become Nambu-Goldstone bosons, but they show unorthodox behavior at small m that $m_\pi^2 = O(m^2)$, which, however, is shown to be consistent with the chiral Ward-Takahashi identities.

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Introduction.—One of possible solutions to the strong CP problem is "massless up quark," where the θ term in QCD can be rotated away by the chiral rotation of up quark without affecting other part of the QCD action. This solution, unfortunately, seems to be ruled out by results from lattice QCD simulations [1].

In a series of papers [2–6], however, one of the present authors has argued that a concept of "massless up quark" is ill-defined if other quarks such as a down quark are all massive, since no symmetry can guarantee masslessness of up quark in this situation due to the chiral anomaly. In addition, it has been also argued that a neutral pion becomes massless at some negative value of up quark mass for the positive down quark mass fixed, and beyond that point, the neutral pion field condenses, forming a spontaneous CP breaking phase, so-called a Dashen phase [7]. Furthermore, at the phase boundary, the topological susceptibility is claimed to diverge due to the massless neutral pion, while it may become zero at the would-be "massless up quark" point.

The purpose of this Letter is to investigate above properties of QCD with nondegenerate quarks in more detail, using the chiral perturbation theory (ChPT) with the effect of anomaly included as the determinant term. For simplicity, we consider the $N_f = 2$ case with $m_u \neq m_d$, but a generalization to an arbitrary number of N_f is straightforward with a small modification. Our analysis explicitly demonstrates the above-mentioned properties such as an absence of any singularity at $m_u = 0$ and the existence of the Dashen phase with the appearance of a massless pion at the phase boundaries. We further apply our analysis to the case of $m_u = m_d = m$ with $\theta = \pi$, which is equivalent to $m_u = -m_d = -m$ with $\theta = 0$ by the chiral rotation. We show that, while η condensation occurs, violating the CP symmetry spontaneously, three pions become Nambu-Goldstone (NG) bosons at $m = 0$ deep in the η condensation phase. We also show a unorthodox behavior at small m that $m_\pi^2 = O(m^2)$, which is indeed shown to be consistent with the chiral Ward-Takahashi identities (WTI).

Phase structure, masses, and topological susceptibility.—The theory we consider in this Letter is given by

$$\mathcal{L} = \frac{f^2}{2}\,\mathrm{tr}(\partial_\mu U \partial^\mu U^\dagger) - \frac{1}{2}\,\mathrm{tr}(M^\dagger U + U^\dagger M) - \frac{\Delta}{2}(\det U + \det U^\dagger), \tag{1}$$

where f is the pion decay constant, M is a quark mass matrix, and Δ is a positive constant giving an additional mass to an eta meson. Differences between an ordinary ChPT and the above theory we consider are the presence of the determinant term [8], which breaks $U(1)$ axial symmetry, thus representing the anomaly effect, and field $U \in U(N_f)$ instead of $U \in SU(N_f)$. We here ignore $\det U$ terms with derivatives for simplicity, since they do not change our conclusions. For $N_f = 2$, without a loss of generality, the mass term is taken as

$$M = e^{i\theta}\begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix} \equiv e^{i\theta} 2B \begin{pmatrix} m_{0u} & 0 \\ 0 & m_{0d} \end{pmatrix}, \tag{2}$$

where B is related to the magnitude of the chiral condensate at the massless limit of the positive degenerate u, d quark masses, thus is positive and mass independent, $m_{0u,0d}$ are

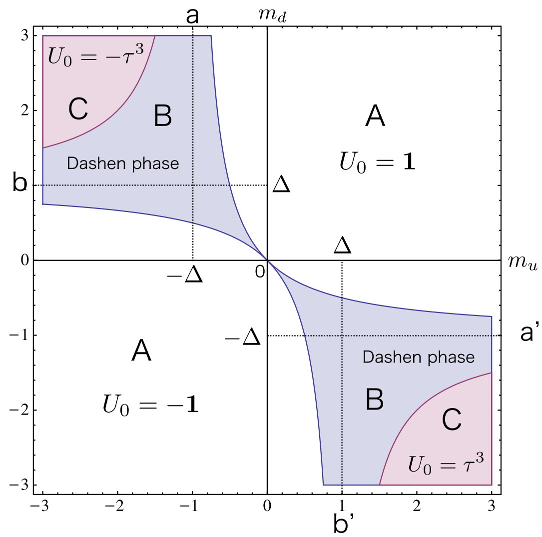

FIG. 1 (color online). Phase structure in m_u-m_d plain, where the CP breaking Dashen phase are shaded in gray (blue), while the CP preserving phase with $U_0 = \tau^3$ (lower right) or $U_0 = -\tau^3$ (upper left) are shaded in light gray (red).

bare quark masses, and θ represents the θ parameter in QCD. We consider that any explicit $F\tilde{F}$ term in the action has been rotated into the mass matrix. In the most of our analysis, we take $\theta = 0$, but an extension of our analysis to $\theta \neq 0$ is straightforward.

Let us determine the vacuum structure of the theory at $m_u \neq m_d$. Minimizing the action with

$$U(x) = U_0 = e^{i\varphi_0} e^{i\sum_{a=1}^{3} \tau^a \varphi_a}, \tag{3}$$

we obtain the phase structure given in Fig. 1, which is symmetric with respect to $m_+ \equiv m_u + m_d = 0$ axis and $m_- \equiv m_d - m_u = 0$ axis, separately. The former symmetry is implied by the chiral rotation that $U \to e^{i\pi\tau^1/2} U e^{i\pi\tau^1/2}$ ($\psi \to e^{i\pi\gamma_5\tau^1/2}\psi$ for the quark), while the latter by the vector rotation that $U \to e^{i\pi\tau^1/2} U e^{-i\pi\tau^1/2}$ ($\psi \to e^{i\pi\tau^1/2}\psi$) [13].

In phase A (white), $U_0 = \mathbf{1}_{2\times 2}$ (upper right) or $U_0 = -\mathbf{1}_{2\times 2}$ (lower left), while $U_0 = \tau^3$ (lower right) or $U_0 = -\tau^3$ (upper left) in phase C [shaded in light gray (red)]. In phase B [shaded in gray (blue)], we have a nontrivial minimum with

$$\sin^2(\varphi_3) = \frac{(m_d - m_u)^2\{(m_u + m_d)^2\Delta^2 - m_u^2 m_d^2\}}{4m_u^3 m_d^3}, \tag{4}$$

$$\sin^2(\varphi_0) = \frac{(m_u + m_d)^2\Delta^2 - m_u^2 m_d^2}{4m_u m_d \Delta^2}, \tag{5}$$

which breaks CP symmetry spontaneously, since $\langle\pi^0\rangle = \mathrm{tr}\tau^3(U_0 - U_0^\dagger)/(2i) = 2\cos(\varphi_0)\sin(\varphi_3)$ and $\langle\eta\rangle = \mathrm{tr}(U_0 - U_0^\dagger)/(2i) = 2\sin(\varphi_0)\cos(\varphi_3)$. This phase, where the neutral pion and the eta fields condense, corresponds to the Dashen phase. The spontaneous CP breaking second-order phase transition occurs at the boundaries of the Dashen phase: Lines between phase A and phase B, on which $\sin^2\varphi_3 = \sin^2\varphi_0 = 0$, are defined by $(m_d + m_u)\Delta + m_d m_u = 0$ (a line $\overline{aa'}$) and $(m_d + m_u)\Delta - m_d m_u = 0$ (a line $\overline{bb'}$), while those between B and C, on which $\sin^2\varphi_3 = \sin^2\varphi_0 = 1$, are given by $(m_d - m_u)\Delta + m_d m_u = 0$ (a line $\overline{ab}$) and $(m_d - m_u)\Delta - m_d m_u = 0$ (a line $\overline{a'b'}$). Note that $\sin^2\varphi_3 = 1$ also on a $m_+ = 0$ line.

We next calculate pseudoscalar (PS) meson masses in each phase. Expanding $U(x)$ around U_0 as $U(x) = U_0 e^{i\Pi(x)/f}$ with

$$\Pi(x) = \begin{pmatrix} \frac{\eta(x)+\pi_0(x)}{\sqrt{2}} & \pi_-(x) \\ \pi_+(x) & \frac{\eta(x)+\pi_0(x)}{\sqrt{2}} \end{pmatrix}, \tag{6}$$

the mass term is given by

$$\mathcal{L}^M = \frac{m_+(\vec{\varphi})}{4f^2}\{\eta^2(x) + \pi_0^2(x) + 2\pi_+(x)\pi_-(x)\} + \frac{\delta m}{2f^2}\eta^2(x) - \frac{m_-(\vec{\varphi})}{2f^2}\eta(x)\pi_0(x), \tag{7}$$

where $m_\pm(\vec{\varphi}) = m_\pm\cos(\varphi_0)\cos(\varphi_3) + m_\mp\sin(\varphi_0)\sin(\varphi_3)$ with $\delta m = 2\Delta\cos(2\varphi_0)$. While the charged meson mass $m_{\pi_\pm}$ is simply given by $m_{\pi_\pm}^2 = m_+(\vec{\varphi})/(2f^2)$, mass eigenstates,

$$\begin{pmatrix} \tilde{\pi}_0(x) \\ \tilde{\eta}(x) \end{pmatrix} = \frac{1}{\sqrt{2X}}\begin{pmatrix} X_+^{1/2}\pi_0(x) + X_-^{1/2}\eta(x) \\ X_-^{1/2}\pi_0(x) - X_+^{1/2}\eta(x) \end{pmatrix}, \tag{8}$$

have

$$m_{\tilde{\pi}_0}^2 = \frac{1}{2f^2}[m_+(\vec{\varphi}) + \delta m - X], \tag{9}$$

$$m_{\tilde{\eta}}^2 = \frac{1}{2f^2}[m_+(\vec{\varphi}) + \delta m + X], \tag{10}$$

where $X = \sqrt{m_-(\vec{\varphi})^2 + \delta m^2}$ and $X_\pm = X \pm \delta m$. We here choose $\tilde{\pi}_0$ and $\tilde{\eta}$ such that $m_{\tilde{\pi}_0}^2 \le m_{\tilde{\eta}}^2$. It is then easy to see $m_{\tilde{\pi}_0}^2 \le m_{\pi_\pm}^2 \le m_{\tilde{\eta}}^2$.

By plugging φ_0 and φ_3 into the above formula, we obtain meson masses in each phase. Here we show that $m_{\tilde{\pi}_0}^2 = 0$ at all phase boundaries, to demonstrate that the phase transition is indeed of second order. In phase A, we have

$$m_{\tilde{\pi}_0}^2 = \frac{1}{2f^2}\left[|m_+| + 2\Delta - \sqrt{m_-^2 + 4\Delta}\right], \tag{11}$$

which becomes zero at $(m_d + m_u)\Delta + m_d m_u = 0$ (on $\overline{aa'}$) and at $(m_d + m_u)\Delta - m_d m_u = 0$ (on $\overline{bb'}$). Note that nothing special happens at $m_u = 0$ (a massless up quark) at $m_d \neq 0$ as $m_{\tilde{\pi}_0}^2 = (|m_d| + 2\Delta - \sqrt{m_d^2 + 4\Delta})/(2f^2)$. In phase C, we obtain

$$m_{\tilde{\pi}_0}^2 = \frac{1}{2f^2}\left[|m_-| - 2\Delta - \sqrt{m_+^2 + 4\Delta}\right], \quad (12)$$

$m_{\tilde{\pi}_0}^2 = 0$ at $(m_d - m_u)\Delta + m_d m_u = 0$ (on $\overline{ab}$) and at $(m_d - m_u)\Delta - m_d m_u = 0$ (on $\overline{a'b'}$). In addition, it is easy to check that the massless condition for $\tilde{\pi}_0$ that $m_+(\vec{\varphi}) + \delta m = \sqrt{m_-(\vec{\varphi})^2 + \delta m^2}$ in phase B can be satisfied only on all boundaries of phase B.

So far, we have shown three claims in Refs. [2–4,6] that (1) the Dashen phase with spontaneous CP breaking by the pion condensate exists in nondegenerate two-flavor QCD, (2) the massless neutral pion appears at the boundaries of the Dashen phase, and (3) nothing special happens at $m_u = 0$ except at $m_d = 0$.

We now consider the relation between the topological susceptibility and m_u in the ChPT. To define the topological susceptibility in ChPT, let us consider the chiral U(1) WTI given by

$$\langle\{\partial^\mu A_\mu^0(x) + \mathrm{tr}M(U^\dagger(x) - U(x)) - 2N_f q(x)\}\mathcal{O}(y)\rangle = \delta^{(4)}(x-y)\langle\delta^0\mathcal{O}(y)\rangle, \quad (13)$$

where $A_\mu = f^2\mathrm{tr}\{U^\dagger(x)\partial_\mu U(x) - U(x)\partial U^\dagger(x)\}$ is the U(1) axial current, $\mathcal{O}$ and $\delta^0\mathcal{O}$ are an arbitrary operator and its infinitesimal local axial U(1) rotation, respectively, and $2N_f q(x) \equiv \Delta\{\det U(x) - \det U^\dagger(x)\}$ corresponds to the topological charge density. Taking $\mathcal{O}(y) = q(y)$ and integrating over x, we define the topological susceptibility in the ChPT through WTI as

$$\begin{aligned} 2N_f\chi &\equiv \int d^4x\langle\{\partial^\mu A_\mu^0(x) + \mathrm{tr}M(U^\dagger(x) - U(x))\}q(y)\rangle, \\ &= \frac{\Delta^2}{4}\int d^4x\langle q(x)q(y)\rangle + \frac{\Delta}{2}\langle\det U(x) + \det U^\dagger(x)\rangle, \end{aligned} \quad (14)$$

where the second term comes from $\delta^0 q(x)$ in ChPT, which is absent in QCD, but represents an effect of the contact term of $q(x)q(y)$ in ChPT. The leading order in ChPT gives

$$2N_f\chi = -\frac{4\Delta^2 m_+(\vec{\varphi})}{m_+(\vec{\varphi})^2 - m_-(\vec{\varphi})^2 + 2m_+(\vec{\varphi})\delta m} + \Delta. \quad (15)$$

At $m_u = 0$, we have $m_+(\vec{\varphi}) = m_-(\vec{\varphi}) = |m_d|$ and $\delta m = 2\Delta$, so that

$$2N_f\chi = -4\Delta^2|m_d|/(4|m_d|\Delta) + \Delta = 0, \quad (16)$$

which confirms the statement that (4) $\chi = 0$ at $m_u = 0$. Since the denominator of χ is proportional to $m_{\tilde{\pi}_0}^2 \times m_{\tilde{\eta}}^2$, $\chi \to -\infty$ on all phase boundaries since $m_{\tilde{\pi}_0}^2 = 0$ and $m_+(\vec{\varphi}) > 0$, which again confirms the statement that (5) χ negatively diverges at the phase boundaries where the neutral pion becomes massless.

We have confirmed the five statements in Refs. [2–4,6], (1)–(5) in the above, by the ChPT analysis. In addition, we have found a new CP preserving phase, phase C, which has $U_0 = \pm\tau^3$ instead of $U_0 = \pm\mathbf{1}_{2\times2}$ of phase A. Since phase C occurs at rather heavy quark masses such that $m_{u,d} = 2Bm_{u,d}^0 = O(\Delta)$, however, the leading-order ChPT analysis may not be reliable for phase C. Indeed, phase C seems to disappear if $(\log\det U)^2$ is employed instead of $\det U$. Other properties, (1)–(5), on the other hand, are robust, since they already occur near the origin ($m_u = m_d = 0$) in the $m_u - m_d$ plain and they survive even if $(\log\det U)^2$ is used.

Property (4) suggests an interesting possibility that one can define $m_u = 0$ at $m_d \neq 0$ in two-flavor QCD from a condition that $\chi = 0$. This is different from the standard statement that the effect of θ term is rotated away at $m_u = 0$. We instead define $m_u = 0$ from $\chi = 0$, which is equivalent to an absence of the θ dependence if higher-order cumulants of topological charge fluctuations are all absent. A question we may have is whether or not $\chi = 0$ is a well-defined condition. Although $\langle q(x)q(y)\rangle$, and thus χ, are notoriously ambiguous due to the short distance divergences, several nonperturbative methods have been proposed and used to calculate χ in lattice QCD [14–16]. As already discussed in Refs. [2–4,6], however, the value of χ, and thus the $\chi = 0$ condition, depends on its definition at finite lattice spacing (cutoff). Although one might naively expect any ambiguity in χ to disappears in the continuum limit, we must check a uniqueness of χ explicitly in lattice QCD calculations by demonstrating that χ from two different definitions but at same physical parameters agree in the continuum limit. If the uniqueness of χ can be established, one should calculate χ at the physical point of $1+1+1$ flavor QCD in the continuum limit. If $\chi \neq 0$ in the continuum limit, the solution to the U(1) problem by the massless up quark ($\chi = 0$ in our definition) is ruled out.

Degenerate two-flavor QCD at $\theta = \pi$.—In the remainder of this Letter, as an application of our analysis, we consider the two-flavor QCD with $m_u = m_d = m$ and $\theta = \pi$, which is equivalent to the two-flavor QCD with $m_u = -m_d$ but $\theta = 0$. In both systems, we have a SU(2) symmetry generated by $\{\tau^1, \tau^2, \tau^3\}$ for the former or $\{\tau^1\gamma_5, \tau^2\gamma_5, \tau^3\}$ for the latter. We here give results for the former case, but a reinterpretation of results in the latter case is straightforward.

The vacuum is given by $\varphi_3 = 0$ and

$$\cos\varphi_0 = \begin{cases} 1, & 2\Delta \le m \\ \frac{m}{2\Delta}, & -2\Delta < m < 2\Delta\,, \\ -1, & m \le -2\Delta \end{cases} \quad (17)$$

which leads to

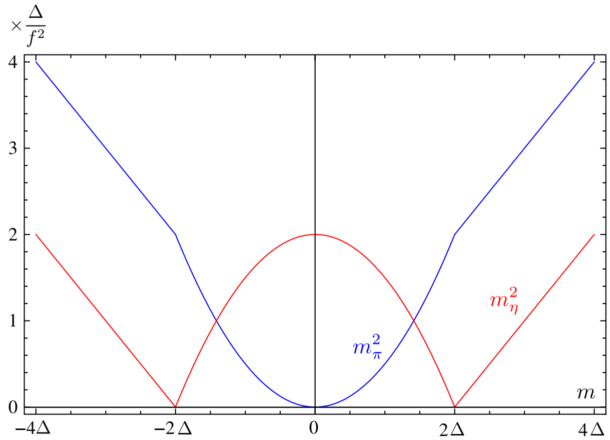

FIG. 2 (color online). m_π^2 [gray (blue)] and m_η^2 [light gray (red)] in unit of $\frac{\Delta}{f^2}$ as a function of m.

$$\langle \bar\psi i\gamma_5\psi\rangle = \begin{cases} 0, & m^2 \geq 4\Delta^2 \\ \pm 2\sqrt{1-\frac{m^2}{4\Delta^2}}, & m^2 < 4\Delta^2 \end{cases}, \quad (18)$$

$$\langle \bar\psi\psi\rangle = \begin{cases} 2, & 2\Delta \leq m \\ \frac{m}{\Delta}, & -2\Delta < m < 2\Delta \\ -2, & m \leq -2\Delta \end{cases}, \quad (19)$$

showing the spontaneous CP symmetry breaking at $m^2 < 4\Delta^2$. Note that $\langle\bar\psi\psi\rangle^2 + \langle\bar\psi i\gamma_5\psi\rangle^2 = 4$ at all m.

PS meson masses are calculated as

$$m_\pi^2 = m_{\pi_\pm}^2 = m_{\pi_0}^2 = \begin{cases} \frac{1}{2f^2}2|m|, & m^2 \geq 4\Delta^2 \\ \frac{1}{2f^2}\frac{m^2}{\Delta}, & m^2 < 4\Delta^2 \end{cases}, \quad (20)$$

$$m_\eta^2 = \begin{cases} \frac{1}{2f^2}[2|m| - 4\Delta], & m^2 \geq 4\Delta^2 \\ \frac{1}{2f^2}\frac{4\Delta^2-m^2}{\Delta}, & m^2 < 4\Delta^2 \end{cases}, \quad (21)$$

where η becomes massless at the phase boundaries at $m^2 = 4\Delta^2$, showing that η is the massless mode associated with the spontaneous CP symmetry breaking phase transition, while three pion become massless Nambu-Goldstone modes at $m = 0$. Figure 2 represents these behaviors.

As mentioned before, although ChPT analysis around the phase transition points at $m^2 = 4\Delta^2$ may not be reliable [17], we can trust the results near $m = 0$ that the CP symmetry is spontaneously broken by the η condensation in the degenerate two-flavor QCD with $\theta = \pi$ and three pions become massless NG bosons at $m = 0$. Pion masses, however, behaves as $m_\pi^2 = m^2/(2f^2\Delta)$ near $m = 0$, contrary to the orthodox PCAC relation that $m_\pi^2 = |m|/(2f^2)$ [18]. Let us show that this unorthodox relation can be explained by the WTI. The integrated WTI for the non-singlet chiral rotation with τ^3 and $\mathcal{O} = \mathrm{tr}\tau^3(U^\dagger - U)$ reads

$$m\int d^4x \mathrm{tr}\tau^3(U^\dagger - U)(x)\mathrm{tr}\tau^3(U^\dagger - U)(y)\rangle = -2\langle \mathrm{tr}(U + U^\dagger)(y)\rangle, \quad (22)$$

which leads to

$$m_{\pi_0}^2 = \frac{m}{f^2}\cos\varphi_0 = \frac{m}{f^2}\frac{m}{2\Delta}. \quad (23)$$

This tells us that one m explicitly comes from the WTI, the other m from the VEV of $\bar\psi\psi$, giving the unorthodox relation,

$$m_\pi^2 = \frac{m^2}{2f^2\Delta}. \quad (24)$$

It is interesting and challenging to confirm this prediction by lattice QCD simulations with $\theta = \pi$, since the weight factor $e^{i\pi Q}$ in the path integral becomes negative for odd integer Q. Furthermore, this new dynamics of non-Abelian gauge theories with fermions might become useful for some particle phenomenologies in the future.

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