Pion masses in 2-flavor QCD with η condensation

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Abstract

We investigate some aspects of 2-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 ChPT 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.

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 non-degenerate 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-Glodstone (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

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

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[15], 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, $m_{0u,0d}$ are 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 straight-forward.

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 $U \to e^{i\pi\tau^1/2}Ue^{i\pi\tau^1/2}$ ($\psi \to e^{i\pi\gamma_5\tau^1/2}\psi$ for the quark), while the latter by the vector rotation that $U \to e^{i\pi\tau^1/2}Ue^{-i\pi\tau^1/2}$ ($\psi \to e^{i\pi\tau^1/2}\psi$)[16].

In the phase A (white), $U_0 = \mathbf{1}_{2\times2}$ (upper right) or $U_0 = -\mathbf{1}_{2\times2}$(lower left), while $U_0 = \tau^3$ (lower right) or $U_0 = -\tau^3$ (upper left) in the phase C (shaded in red). In the phase B (shaded in blue), we have nontrivial minimum with

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

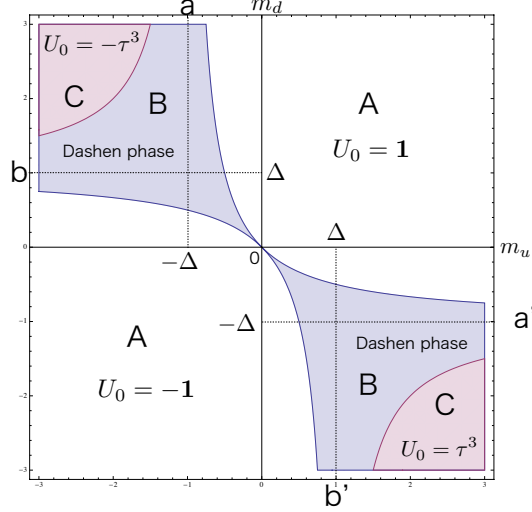$$\sin^2(\varphi_0) = \frac{(m_u + m_d)^2\Delta^2 - m_u^2 m_d^2}{4m_u m_d \Delta^2}, \tag{5}$$

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

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 2nd-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 pseudo-scalar meson masses in each phase. Expanding $U(x)$ around U_0 as $U(x) = U_0 e^{i\Pi(x)/f}$ with

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

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the mass term is given by

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

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

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

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

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 the 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 the phase C, we obtain

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

$m_{\tilde{\pi}_0}^2 = 0$ 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 the phase B can be satisfied only on all boundaries of the phase B.

So far, we have shown three claims in [2–4, 6] that (1) the Dashen phase with spontaneous CP breaking by the pion condensate exists in non-degenerate 2-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

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

where $A_\mu = f^2 \operatorname{tr}\{U^\dagger(x)\partial_\mu U(x) - U(x)\partial U^\dagger(x)\}$ 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

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

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

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

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

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

which confirms the statement that (4) $\chi = 0$ at $m_u = 0$. Since the denominator of χ is proportional to $m_{\pi_0}^2 \times m_{\hat{\eta}}^2$, $\chi \to -\infty$ on all phase boundaries since $m_{\pi_0}^2 = 0$ 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 Ref. [2–4, 6], (1) – (5) in the above, by the ChPT analysis. In addition, we have found a new CP preserving phase, the phase C, which has $U_0 = \pm\tau^3$ instead of $U_0 = \pm\mathbf{1}_{2\times 2}$ of the phase A. Since the 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 the phase C. Indeed, the 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.

The property (4) suggests an interesting possibility that one can define $m_u = 0$ at $m_d \neq 0$ in 2-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 $\chi = 0$ is a well defined condition or not. As already discussed in Ref. [2–4, 6], a value of χ, and thus the $\chi = 0$ condition, depend on its definition at finite lattice spacing (cut-off). Although one naively expect such ambiguity of χ 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 2-FLAVOR QCD AT $\theta = \pi$

In the remainder of this letter, as an application of our analysis, we consider the 2-flavor QCD with $m_u = m_d = m$ and $\theta = 0$, which is equivalent to the 2-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

$$
\cos \varphi_0 = \begin{cases} 1, & 2\Delta \leq m \\ \dfrac{m}{2\Delta}, & -2\Delta < m < 2\Delta \\ -1, & m \leq -2\Delta \end{cases} , \tag{17}
$$

which leads to

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

$$\langle \bar{\psi} \psi \rangle = \begin{cases} 2, & 2\Delta \leq m \\ \dfrac{m}{\Delta}, & -2\Delta < m < 2\Delta \\ -2, & m \leq -2\Delta \end{cases}, \tag{19}$$

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

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

$$m_\eta^2 = \begin{cases} \dfrac{1}{2f^2} \left[2|m| - 4\Delta \right], & m^2 \geq 4\Delta^2 \\ \dfrac{1}{2f^2} \dfrac{4\Delta^2 - m^2}{\Delta}, & m^2 < 4\Delta^2 \end{cases}, \tag{21}$$

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 $m = 0$. Fig. 2 represents these behaviors.
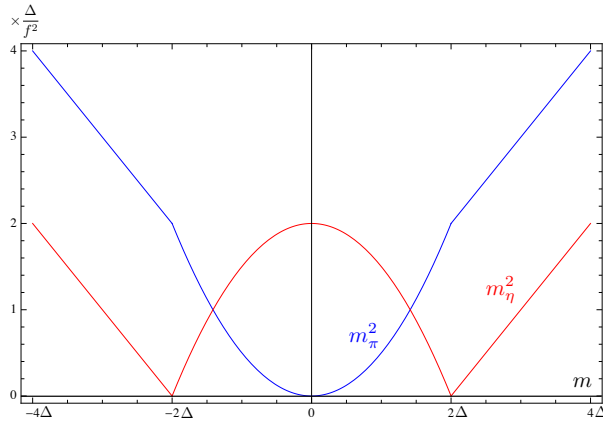

FIG. 2: m_π^2 (blue) and m_η^2 (red) in unit of $\frac{\Delta}{f^2}$ as a function of m.

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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 2-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 $\mathcal{O} = \operatorname{tr}\tau^3(U^\dagger - U)$ reads

$$
\begin{aligned}
m \int d^4x \operatorname{tr}\tau^3(U^\dagger - U)(x)\operatorname{tr}\tau^3(U^\dagger - U)(y)\rangle \\
= -2\langle\operatorname{tr}(U + U^\dagger)(y)\rangle,
\end{aligned}
\tag{22}
$$

which leads to

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

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 that

$$
m_\pi^2 = \frac{m^2}{2f^2\Delta}.
\tag{24}
$$

It is interesting and challenging, because of sign problems, to confirm this prediction by lattice QCD simulations with $\theta = \pi$, and to consider possible applications of this to particle physics [7].

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[15] Based on the large N behavior, it is standard to use $(\log \det U)^2$ term to incorporate anomaly effects into ChPT[8–11]. Since we can determine the phase structure only numerically in this case, we instead employ $\det U$ term in our analysis, which leads to he phase structure determined analytically. We have checked that the two cases lead to a qualitatively similar phase structure except at large quark masses.

[16] This phase structure seems incompatible with the 1+1 flavor QCD with rooted staggered quarks, which is symmetric individually under $m_u \to -m_u$ or $m_d \to -m_d$. This suggests that the rooted trick for the staggered quarks can not be used in a region at $m_d m_u < 0$.

[17] Indeed, both CP preserving phase, which correspond to the phase C, and the phase transition points, disappear if $(\log \det U)^2$ term is employed instead of $\det U$ term. In this case CP is broken at all m.

[18] A similar behavior has been predicted in a different context[12–14].