QCD at $\theta\sim\pi$ reexamined: Domain walls and spontaneous CP violation

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We consider QCD at $\theta\sim\pi$ with two, one and zero light flavors N_f, using the Di Vecchia–Veneziano–Witten effective Lagrangian. For $N_f=2$, we show that CP is spontaneously broken at $\theta=\pi$ for finite quark mass splittings, $z=m_d/m_u\neq 1$. In the $z-\theta$ plane, there is a line of first order transitions at $\theta=\pi$ with two critical end points, $z_1^*<z<z_2^*$. We compute the tension of the domain walls that relate the two CP violating vacua. For $m_u=m_d$, the tension of the family of equivalent domain walls agrees with the expression derived by Smilga from chiral perturbation theory at next-to-leading order. For $z_1^*<z<z_2^*$, $z\neq 1$, there is only one domain wall and a wall-some sphaleron at $\theta=\pi$. At the critical points, $z=z_{1,2}^*$, the domain wall fades away, CP is restored and the transition becomes of second order. For $N_f=1$, CP is spontaneously broken only if the number of colors N_c is large and/or if the quark is sufficiently heavy. Taking the heavy quark limit ($\sim N_f=0$) provides a simple derivation of the multibranch θ dependence of the vacuum energy of large N_c pure Yang-Mills theory. In the large N_c limit, there are many quasistable vacua with a decay rate $\Gamma\sim\exp(-N_c^4)$.

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I. INTRODUCTION

In the limit of N_f massless quarks, QCD has a global $SU(N_f)\times SU(N_f)$ chiral symmetry. In vacuum, this symmetry is spontaneously broken to the diagonal $SU(N_f)$, with N_f^2-1 massless Goldstone bosons. Introducing quark masses lifts the degeneracy of the vacuum and gives mass to the Goldstone bosons. In addition to the quark masses, there is another parameter in QCD, known as theta (θ). In nature, $\theta\sim 0$ modulo 2π. A nonzero value of θ would introduce explicit CP violation in the strong interactions, with decay processes such as $\eta'\to\pi\pi$, or large contributions to the electric dipole moment of the neutron—phenomena which are not observed [1]. Although large values of θ are excluded experimentally, it is fruitful to investigate how strong interactions change for $\theta\neq 0$. A beautiful example is the Veneziano-Witten formula which relates, in the limit of large number of colors N_c, the mass of the η' meson to the second derivative with respect to θ of the vacuum energy of pure Yang-Mills theory [2,3].

We will focus here on the fascinating, but unfortunately academic possibility of spontaneous CP violation at $\theta=\pi$, also known as Dashen's phenomenon [4]. Strong interactions are *a priori* invariant under CP at $\theta=\pi$. This is because $\theta=\pi\to-\pi$ under a CP transformation but physics should be unchanged for $\theta\to\theta+2\pi$, so that $\pi\equiv-\pi$. However, as shown by Dashen some time before the advent of QCD, CP can be spontaneously broken at $\theta=\pi$, with the appearance of two CP violating degenerate vacua separated by a potential energy barrier [4]. According to the Vafa-Witten theorem, this possibility is excluded at $\theta=0$ [5,6]. In the vicinity of $\theta=\pi$, one of the vacua has lower energy and, as θ varies, there is a first order transition at $\theta=\pi$. This phenomenon and related issues has been investigated by Di Vecchia and Veneziano [7] and Witten [8] in the large N_c limit, and more recently by Creutz [9], Evans *et al.* [10] and Smilga [11].

The realistic case of three light flavors has been the most discussed. Di Vecchia and Veneziano [7] and Witten [8] have shown that there are two degenerate vacua at $\theta=\pi$, provided the following constraint is satisfied:

$$\frac{m_u m_d}{m_s}>|m_d-m_u|. \tag{1.1}$$

To our knowledge, the equivalent of Eq. (1.1) for two light flavors has never been published, presumably because this question is *a priori* academic, as the inequality (1.1) is not satisfied for realistic quark masses. (In nature, $m_u\approx 4$ MeV, $m_d\approx 7$ MeV and $m_s\approx 150$ MeV.) The two flavor case is however quite interesting. On one hand, taking the limit $m_s\to\infty$ in Eq. (1.1) seems to imply that CP can only be broken for $m_u=m_d$, which is in agreement with the result found by Di Vecchia and Veneziano [7]. On the other hand Creutz [9] and Evans *et al.* [10] found evidences of CP violation also for finite mass splittings, $z\equiv m_d/m_u\neq 1$. The latter possibility is more natural. In the $z-\theta$ plane, we would expect a line of first order phase transitions at $\theta=\pi$, terminated with critical endpoints $z=z^*$, where the phase transition becomes of second order. A related issue, recently addressed by Smilga [11], is that to leading order in chiral perturbation theory (χPT) the potential term in

$$\mathcal{L}=\frac{f_\pi^2}{4}\mathrm{tr}(\partial_\mu U^\dagger\partial^\mu U)+\Sigma\ \mathrm{Re}[\mathrm{tr}(\mathcal{M}\,e^{i\theta/2}\,U^\dagger)], \tag{1.2}$$

where U is an $SU(2)$ unitary matrix and with

$$\mathcal{M}=\begin{pmatrix} m_u & 0\\ 0 & m_d\end{pmatrix}, \tag{1.3}$$

vanishes at $\theta=\pi$ for $m_u=m_d$. This would imply that pion excitations are massless at $\theta=\pi$, with a second order phase transition while it is expected to be of first order. Within χPT, the paradox is resolved by taking into account next-to-leading order corrections in the quark mass $\mathcal{O}(m^2)$, which lift the vacuum degeneracy at $\theta=\pi$ [11]. However, it is not manifest how precisely this is related to the phenomenon of spontaneous CP violation.

Our contribution will be to draw a self-consistent picture of Dashen's phenomenon at $\theta=\pi$ for the case of two, one and zero light quark flavors. Incidentally, most (but not all) of the results we will discuss can be found scattered in the litterature cited above, either explicitly or implicitly. We will work within the framework of the large N_c Di Vecchia–Veneziano–Witten effective Lagrangian [7,8,12].

For $N_f=1$, CP is spontaneously broken at $\theta=\pi$ only in the very large N_c limit or, alternatively, if the quark is sufficiently heavy. Increasing further the quark mass provides a simple derivation, within field theory, of the peculiar θ dependence of pure Yang-Mills theory at large N_c. Recently, Witten [13] has used the correspondence between large N_c Yang-Mills theories and string theories on some particular compactified spacetimes to *derive* the qualitative form of the vacuum energy [14]. (See also [15–17].) Turning to $N_f=2$, we will show that CP is spontaneously broken with a first order transition at $\theta=\pi$ for a finite range of quark mass splittings, $z_1^*<m_d/m_u<z_2^*$, and will determine the critical values $z_{1,2}^*$ in the limit $m_\pi^2\ll m_{\eta'}^2$. We will compute the tension of the domain walls relating the two CP violating vacua and, in the degenerate limit $z=1$, will recover the result derived by Smilga from chiral perturbation theory at next-to-leading order. At the critical points $z=z_{1,2}^*$, the degenerate vacua merge and the domain wall disappears, CP is restored and the phase transition becomes of second order. Chiral perturbation theory at leading order simply corresponds to the particular limit in which $z_1^*=z_2^*=1$.

II. DOMAIN WALLS AND SPONTANEOUS CP VIOLATION AT $\theta=\pi$

In the large N_c limit, the effects of the $U(1)_A$ anomaly fade away and the η' meson becomes light. In particular, at infinite N_c and in the chiral limit, the η' is massless and there are N_f^2 Goldstone bosons. The phenomenological Lagrangian that incorporate both quark mass and leading large N_c effects is [7,8,12]

$$\mathcal{L}=\frac{f_\pi^2}{4}\mathrm{tr}(\partial_\mu U^\dagger\partial^\mu U)+\Sigma\ \mathrm{Re}[\mathrm{tr}(\mathcal{M}U^\dagger)]$$
$$-\frac{\tau}{2}(\theta+i\log\det U)^2, \tag{2.1}$$

where, specializing to two light flavors, $\mathcal{M}$ is the diagonal quark mass matrix (1.3), $\Sigma=|\langle\overline{q}q\rangle|$ and τ is the topological susceptibility of pure Yang-Mills theory. [In the real world, $\tau\sim(200\text{ MeV})^4$.] Because the mass matrix is diagonal, we can write the vacuum expectation value of the $U(2)$ matrix U in the form

$$U=\begin{pmatrix} e^{i\phi_u} & 0\\ 0 & e^{i\phi_d}\end{pmatrix}. \tag{2.2}$$

If $m_u=m_d$, the choice (2.2) for the vacuum expectation value of the unitary matrix U is one among a whole manifold [with topology $SU(2)/U(1)\sim S^2$] of equivalent ones. This degeneracy is lifted for any $m_u\neq m_d$. We further decompose the phases $\phi_{u,d}$ as

$$\phi_u=\phi+\alpha,$$

$$\phi_d=\phi-\alpha,$$

so that $\log\det U=2i\phi$. The phase ϕ is then related to the vacuum expectation value of the η' field

$$\phi=\langle\eta'\rangle/f_\pi, \tag{2.3}$$

while α is the vacuum expectation value of the π_0 field. Also, in the chiral limit $m_u=m_d=0$,

$$f_\pi^2 m_{\eta'}^2=4\tau, \tag{2.4}$$

which is the celebrated Veneziano-Witten relation for two flavors [2,3].

In this basis, the potential energy term of Eq. (2.1) reads

$$\begin{aligned}E(\theta)&=-\Sigma m_u\cos(\phi+\alpha)-\Sigma m_d\cos(\phi-\alpha)+\frac{\tau}{2}(\theta-2\phi)^2\\ &=-(m_u+m_d)\Sigma\cos\phi\cos\alpha\\ &\quad+(m_u-m_d)\Sigma\sin\phi\sin\alpha+\frac{\tau}{2}(\theta-2\phi)^2.\end{aligned} \tag{2.5}$$

Minimizing $E(\theta)$ with respect to ϕ and α gives the two equations

$$(m_u+m_d)\cos\phi\sin\alpha+(m_u-m_d)\sin\phi\cos\alpha=0, \tag{2.6}$$

$$(m_u+m_d)\sin\phi\cos\alpha+(m_u-m_d)\cos\phi\sin\alpha=\frac{2\tau}{\Sigma}(\theta-2\phi). \tag{2.7}$$

For generic quark masses and $\theta\neq0,\pi$, the solutions of Eqs. (2.6)–(2.7) are CP violating.

A. General remarks

If m_d goes to zero, Eq. (2.6) gives $\phi+\alpha=0$ modulo π, while Eq. (2.7) imposes $\phi=\theta/2$. (If $m_u\to0$ instead, $\phi-\alpha=0$. In the sequel, we will keep m_u fixed and vary m_d.) In essence, θ has been absorbed in the redefinition of the phase ϕ_d (which is unconstrained by the potential if $m_d=0$), and, as expected, there is no CP violation. Another way to phrase this is that

$$\overline{\theta}=(\theta-2\phi)\quad\text{modulo}\quad\pi \tag{2.8}$$

give the measure of CP violation in strong interactions.[1]

In the opposite limit of a decoupling heavy quark, $m_d \to\infty$, Eq. (2.6) imposes $\alpha=\phi$. Substituting Eq. (2.6) in Eq. (2.7) with $\alpha=\phi$, and redefining $\tilde{\phi}=2\phi$, gives

$$2\Sigma m_u \sin(\tilde{\phi})=2\tau(\theta-\tilde{\phi}). \qquad (2.11)$$

This minimizes

$$E(\theta)=-m_u\Sigma\cos\tilde{\phi}+\frac{\tau}{2}(\theta-\tilde{\phi})^2, \qquad (2.12)$$

which is the potential energy for $N_f=1$, as expected. These limits, $m_d\to 0$ and $m_d\to\infty$, illustrate that the dependence in θ (i.e., CP violation) is controlled by the lightest quark flavor.

B. One and zero flavor

We begin with the analysis of the one flavor case (2.12), which is analogous to the (bosonized) massive Schwinger model in two dimensions [18]. At $\theta=0$, Eq. (2.11) gives (dropping the tilde)

$$\sin\phi=-\frac{\tau}{m_u\Sigma}\phi, \qquad (2.13)$$

which is trivially satisfied for $\phi=0$. This solution is the true ground state and is CP conserving, in agreement with the Vafa-Witten theorem [5]. Other solutions are possible if

$$\tau/m\Sigma\lesssim 2/3\pi. \qquad (2.14)$$

These are CP violating, but metastable (see Fig. 1). At fixed m_u, the condition (2.14) can be satisfied in the very large N_c limit, because $\Sigma=\mathcal{O}(N_c)$, if m_u increases or if $\tau=\mathcal{O}(N_c^0)$ diminishes (dramatically) with respect to its phenomenological value. The first case has been discussed by Witten [8]. The latter possibility has been raised in the context of the deconfining phase transition in QCD at finite temperature [19]. Finally, changing the mass quark allows to change the number of light flavors, as exemplified in the previous section.

At $\theta=\pi$, the trivial, CP conserving solution is $\phi=\pi$. Spontaneous CP violation can occur only if

$$\tau\lesssim m_u\Sigma, \qquad (2.15)$$

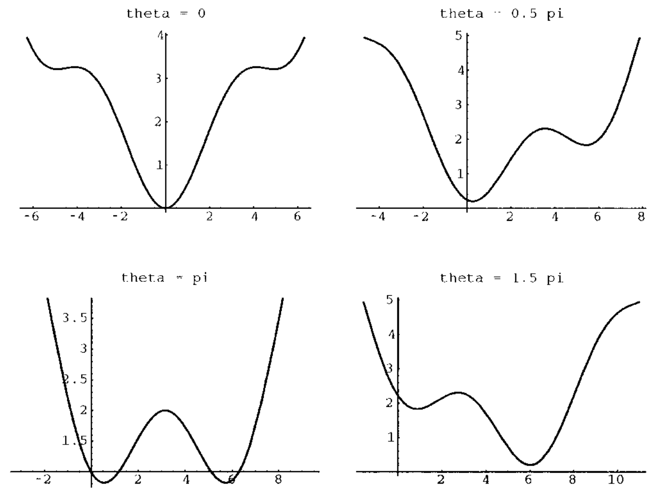

FIG. 1. Potential energy for $N_f=1$ as function of the VEV of η', ϕ. For $m\Sigma\gtrsim\tau$, there are two metastable CP violating solutions at $\theta=0$. At $\theta=\pi$, there are two degenerate vacua CP violating vacua. At $\theta=2\pi$, the potential is the same as at $\theta=0$, but shifted by 2π. (See Fig. 2.)

in which case the CP conserving solution becomes a maximum (see Fig. 1). The inequality (2.15) is the equivalent of Eq. (1.1) for $N_f=1$. At $\theta=2\pi$, things are the same as at $\theta=0$, but with ϕ shifted by 2π. Thus, despite the presence of the term quadratic in θ in the potential energy (2.12), the ground state energy is 2π periodic, simply because a shift like $\theta\to\theta+k2\pi$ is reabsorbed in $\phi\to\phi+k2\pi$.

It may actually be worthwhile to emphasise that the Di Vecchia–Veneziano–Witten effective Lagrangian is consistent not only with the θ dependence of QCD but *also* of pure Yang-Mills theory. If we formally increase m_u, the system indeed shares some resemblance with the limit of zero quark flavor. In particular, this limit provides a very simple derivation of the peculiar θ dependence of large N_c pure Yang-Mills theory. Recently, Witten [13] has derived the vacuum energy using the correspondence between large N_c Yang-Mills theory and string theory on a certain space-time background [14]. (See also Shifman [15] and Gabadadze [17] for a discussion in a field theory context.) The energy has a multibranch structure

$$E(\theta)=N_c^2\min_k F\left(\frac{\theta+k2\pi}{N_c}\right), \qquad (2.16)$$

where k is an integer and

$$F\left(\frac{\theta}{N_c}\right)=C_0+\frac{\tau}{2}\frac{\theta^2}{N_c^2}+\mathcal{O}\left(\frac{\theta^4}{N_c^4}\right). \qquad (2.17)$$

This form of the energy has been postulated by Witten many years ago [3] in order to reconcile large N_c with the requisite 2π periodicity in θ. A striking feature of Eq. (2.16) is that, at fixed θ, it implies the existence of many nondegenerate vacua in pure Yang-Mills theory at large N_c. It has been argued in [8], and explicitely shown in the more recent [13] and [15], that these states are stable at infinite N_c. For com-

[1]To see this, let U_0 be the vacuum expectation of the U matrix, and define $U=U_0V$, $\bar{\mathcal{M}}=\mathcal{M}U_0=\mathcal{A}+i\mathcal{B}$. As shown by Witten [8], vacuum stability requires

$$\Sigma\mathcal{B}=2\tau\bar{\theta}\mathbf{1}_2. \qquad (2.9)$$

With this decomposition and using Eq. (2.9), the CP violating part of the potential (2.1) is

$$E(\theta)_{CP}=-i\tau\bar{\theta}[2\,\mathrm{tr}\,(\mathrm{Im}\,V)-\log\det V] \qquad (2.10)$$

which vanishes if $\bar{\theta}=0$.

pleteness, we show how this conclusion, as well as the large N_c scaling of the quantities of interest, can be reproduced within the framework of the Di Vecchia–Veneziano–Witten effective Lagrangian.

For $m_u\Sigma \gg \tau$, the potential has a large number, $k_{\max} \sim m\Sigma/\tau \sim N_c$, of local minima. At $\theta=0$, the ground state is unique and CP conserving, $\phi_0=0$. Then there are two adjacent, degenerate, metastable solutions

$$\phi_1^{\pm} \approx \pm 2\pi(1-\tau/m\Sigma), \tag{2.18}$$

with energy

$$\Delta E_1 \approx 2\pi^2\tau, \tag{2.19}$$

where we have substracted the trivial contribution from the quark mass term. For generic θ and $k \ll k_{\max}$, $\phi_{\pm} \approx \pm 2k\pi$, with $\Delta E_k \approx (\tau/2)(\theta - k2\pi)^2$. As θ increases from 0, ϕ_0 and the ϕ_k^- go up and the ϕ_k^+ go down. At $\theta=\pi$, $\phi_0 \approx \pi\tau/m\Sigma$ and $\phi_1 \approx 2\pi - \pi\tau/m\Sigma$ become degenerate. In this picture, CP is spontaneously broken at $\theta=\pi$, but only very slightly as $\overline{\theta} \approx \pm 2\pi\tau/m\Sigma$ modulo π, which goes to zero as m or N_c go to infinity. The height of the potential barrier between the two vacua is $m\Sigma \sim N_c$ and they can be related by a domain wall.[2] The profile of the domain wall can be easely estimated in the limit $\tau \ll m\Sigma$. Choosing $\phi(x)=\phi_0=0+\mathcal{O}(\tau/m\Sigma)$ at spatial $x=-\infty$ and $\phi(+\infty)=\phi_1=2\pi+\mathcal{O}(\tau/m\Sigma)$ and solving the differential equation for the phase $\phi(x)$,

$$f_\pi^2\partial_x^2\phi - \delta_\phi E(\phi)=0, \tag{2.20}$$

where E is given by Eq. (2.12), we find

$$\phi(x) \approx \pi + 2\,\arctan\left\{\frac{\exp(\sqrt{m\Sigma}x/f_\pi)-1}{\exp(\sqrt{m\Sigma}x/f_\pi)+1}\right\}. \tag{2.21}$$

In the same approximation, the tension of this domain wall is

$$\sigma=\int_{-\infty}^{+\infty}dx\left\{\frac{1}{2}f_\pi^2(\partial_x\phi)^2+E(\phi)\right\} \approx 8f_\pi\sqrt{m\Sigma} \sim N_c. \tag{2.22}$$

Let us comment about the validity of these expressions, Eqs. (2.21) and (2.22). Note that the domain wall configuration arises from the balance between the kinetic and quark mass terms, which are of the same order in the low energy expansion of the effective theory.[3] From Eq. (2.21), the domain wall has a width $\delta \approx f_\pi/\sqrt{m\Sigma} \sim 1/M$, where $M \sim N_c^0$ is the meson mass, so that the gradient of the meson field is typically $\mathcal{O}(M/f_\pi)$ accross the wall. Corrections to the leading order results (2.21) and (2.22) from higher order operators are thus under control as long as we keep $M \ll f_\pi$, which imposes the following hierarchy $\tau \ll m\Sigma \equiv M^2 f_\pi^2 \ll f_\pi^4$.

Increasing θ further, $\phi \approx 0$ becomes a local minimum while $\phi \approx 2\pi$ becomes the true ground state. When θ reaches 2π, things just repeat, with ϕ shifted by 2π. If we integrate out the heavy quark, the ground state energy as function of θ becomes

$$\begin{aligned} E(\theta) &= \frac{\tau}{2}\min_\phi(\theta-\phi)^2 \\ &\approx \frac{\tau}{2}\min_k(\theta-2k\pi)^2, \end{aligned}$$

which agrees with the multibranch structure of (2.16) and shows that the Di Vecchia-Veneziano-Witten is (at least formally) consistent with the expected θ dependence of pure Yang-Mills theory at large N_c.[4]

At fixed θ there is a large number of metastable states, corresponding to $\phi \approx k2\pi$.[5] (See Figs. 1 and 2.) For k large, $k \lesssim k_{\max}$, these states are essentially unstable. For small $k \ll k_{\max}$, the lifetime of the lowest lying solutions can be easely evaluated. The energy difference between two adjacent ($\Delta k=1$) vacua $\Delta E \approx 2\tau\pi^2 \sim N_c^0$ is much less than the eight of the potential barrier, $E \approx m\Sigma \sim N_c$ and the thin-wall approximation applies [21,22]. The decay rate is $\Gamma \exp(-S_E)$, where S_E is the Euclidean action for a bubble of lower energy vacuum. In the thin wall approximation, S_E is well approximated by

$$S_E \approx -\pi^4\tau\frac{R^4}{4}+2\pi^2R^3\sigma, \tag{2.23}$$

where the first term is the contribution from the volume and the other from the surface tension (2.22), while R is the radius of the bubble of ''true'' vacuum. The action S_E (2.23) is extremized for

$$R_c \approx \frac{6\sigma}{\pi^2\tau} \sim N_c. \tag{2.24}$$

while from Eq. (2.21), the bubble wall thickness is $\delta \sim f_\pi/\sqrt{m\Sigma} \sim N_c^0 \ll R_c$. The rate for a (low lying) false vacuum to decay to its lower energy neighbor is finally given by

[2]In the AdS conformal field theory (CFT) approach, the domain wall is a wrapped six-brane (with $\sigma \sim N_c$). In the $N=1$ SUSY approach, the domain wall relates two adjacent vacua, out of the Z_{N_c} distinct ones with different gluino condensate.

[3]The situation is thus better than for skyrmions. The stability of these topological defects necessitates to mix different orders in the low energy expansion, while in the case of domain walls the calculations can be made arbitrarily reliable, even in an effective theory.

[4]For *this* particular matter, the modifications of the Di Vecchia–Veneziano–Witten effective Lagrangian proposed in [20] thus seem superfluous.

[5]In this picture, $\langle\phi\rangle$ is a sort of auxiliary field which labels the different vacua branches. It plays a role similar to the gluino condensate in $N=1$ supersymmetry (SUSY) or to the flux of the $U(1)$ gauge field from the Ramond-Ramond sector of type IIA superstring in the AdS-CFT correspondence.

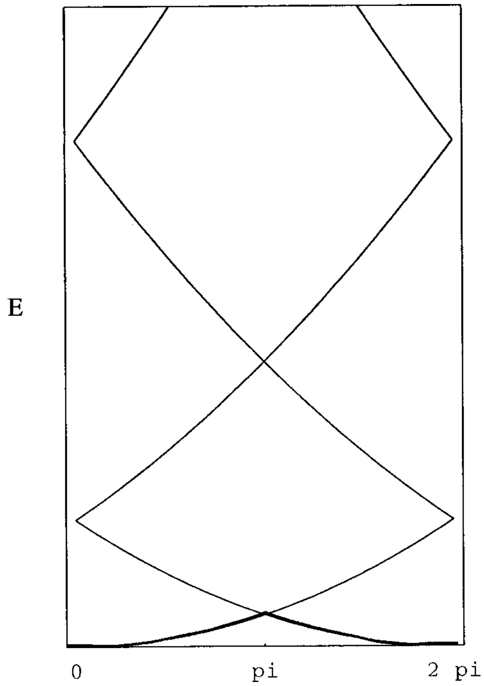

FIG. 2. Energy levels for $m\Sigma \gg \tau$ ($\sim N_f=0$) and $0\leqslant\theta<2\pi$ (first Brillouin zone). For fixed θ, there are many *metastable* vacua, corresponding to $\langle\phi\rangle\approx k2\pi$. At $\theta=\pi$, the lowest energy levels cross and there are two degenerate vacua. (See Fig. 1.)

$$\Gamma\sim\exp\left(-\frac{272^8 f_\pi^4 m^2\Sigma^2}{\pi^4\tau^3}\right)\sim\exp(-N_c^4) \qquad (2.25)$$

so that, as N_c goes to infinity, the non-degenerate vacua become stable.

Shifman has also attempted to compute the decay rate of the lowest lying metastable states in the pure Yang-Mills theory, but starting from $N=1$ super Yang-Mills (SYM) theory and decoupling the gluinos [15]. (See also Gabadadze [17].) His expression, which rests on the (well motivated) assumption that the domain walls relating adjacent vacua in $N=1$ SYM theory are Bogomol'nyi-Prasad-Sommerfield (BPS) saturated states, is reliable for small gluinos masses, *i.e.* m_g smaller than $|\langle\lambda\lambda\rangle|=\Lambda$ where $\langle\lambda\lambda\rangle$ is the gluino condensate. Similarly, the expression we have derived, Eq. (2.25), is valid as long as chiral perturbation theory is reliable, that is if the quark mass is such that $M^2\ll f_\pi^2$, where M is the meson mass. In order to match to the pure glue theory requires to decouple respectively the gluinos or the heavy quark. In the former case, one loses the control of holomorphy, while in the latter case chiral perturbation theory breaks down. As could be expected, the predictions of $N=1$ SYM theory and of chiral perturbation theory can only be compared at a qualitative level. It is quite remarkable that the N_c scaling of the decay rate, Eq. (2.25), is precisely the same in both approaches.

C. Two flavors, degenerate case

If $m_u=m_d\equiv m$, the equations (2.6),(2.7) can be easily solved at $\theta=\pi$, at least in the limit $m\Sigma\ll\tau$, which we will assume to hold from now on. Defining $\phi=\pi/2+\varphi$, the potential energy (2.5),

$$E(\theta)=-2m\Sigma\cos\phi\cos\alpha+\frac{\tau}{2}(\theta-2\phi)^2, \qquad (2.26)$$

becomes

$$E(\pi)=2m\Sigma\sin\varphi\cos\alpha+2\tau\varphi^2 \qquad (2.27)$$

and Eqs. (2.6),(2.7),

$$\sin\varphi\sin\alpha=0, \qquad (2.28)$$

$$\cos\varphi\cos\alpha=-2\frac{\tau}{m\Sigma}\varphi. \qquad (2.29)$$

Note first that if $\tau/m\Sigma\to\infty$, $\varphi=0$, and CP is not broken ($\bar{\theta}\equiv 2\varphi=0$). The potential (2.27) vanishes for any α—the pion are massless, and the transition at $\theta=\pi$ is of second order. This is precisely the situation that occurs to leading order in $SU(2)\times SU(2)$ χPT and raised as a puzzle by Smilga [11]. Integrating out the η' from Eq. (2.26) in the limit $\tau/m\Sigma\to\infty$, sets $\phi\equiv\theta/2$ and gives

$$E(\theta)=-2m\Sigma\cos\frac{\theta}{2}\cos\alpha, \qquad (2.30)$$

which is the potential energy to leading order in χPT. At $\theta=\pi$, Eq. (2.30) vanishes.

In the limit $m\Sigma\ll\tau$, it is easy to solve the equations (2.6). The trivial CP conserving solution is

$$\varphi_I=0, \quad \alpha_I=\pi/2 \quad \text{modulo} \quad \pi. \qquad (2.31)$$

This solution is however a saddle point, with $E_I=0$. The true ground state is CP violating, with the two solutions

$$\begin{aligned}\varphi_{II}&\approx-m\Sigma/2\tau, \quad \alpha_{II}=0,\\ \varphi_{III}&\approx m\Sigma/2\tau, \quad \alpha_{III}=\pi,\end{aligned} \qquad (2.32)$$

and

$$E_{II}=E_{III}\approx-\frac{m^2\Sigma^2}{2\tau}. \qquad (2.33)$$

Contrary to the one flavor case (2.15), for $N_f=2$ spontaneous CP violation occurs for any *finite* $\tau/m\Sigma$.

The two CP violating vacua are separated by an energy barrier (see Fig. 3 with $z=1$) and can be related by a domain wall. Note that for $m_u=m_d$ the vacuum has an $SU(2)/U(1)\sim S^2$ degeneracy and, correspondingly, there is an infinite family of domain walls with the same tension. Two of these vacua are shown in Fig. 3, $z=1$. The vacua at $\alpha=0$ and $\alpha=2\pi$ as well as the saddle points at $\alpha=\pi/2$ and $\alpha=3\pi/2$ are equivalent and can be mapped onto each other by a Weyl reflection, $\alpha\to-\alpha$ (modulo 2π). This degeneracy is lifted for any $m_u\neq m_d$: there are only *two* vacua, which are shown in Fig. 3 for $z\neq1$, and *one* domain wall [11]. As discussed in the next section, there is also a wall-

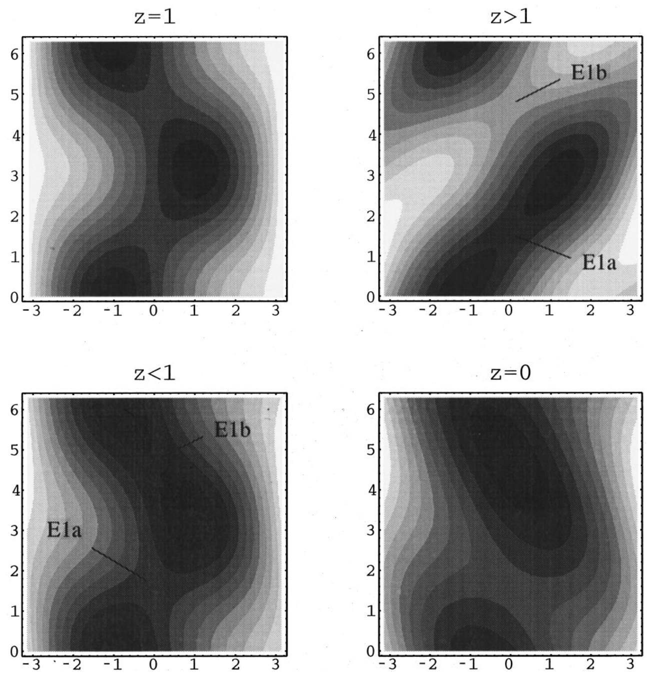

FIG. 3. These figures show contour plots of the potential energy for the case of two quark flavors at $\theta=\pi$. The vacuum expectation of the η' field, $\varphi=\phi-\pi/2$, is plotted on the horizontal axis. The CP violating vacua correspond to the dark spots with $\varphi\neq 0$. The VEV of the pion field, α, is plotted on the vertical axis. (We have taken $m\Sigma\sim\tau$ to make the picture more impressive.) At $z=1$ ($m_u=m_d$) there are two CP violating vacua, separated by an energy barrier. Note that the vacua at $\alpha\sim 2\pi$ and $\alpha\sim 0$ are *identical*. In this degenerate limit, there is an infinite family of equivalent vacua, related by an infinite number of equivalent domain wall configurations. At $z\neq 0$, this degeneracy is lifted and there are only two vacua. Consider $z>1$ for definitiveness. The configuration which interpolates between the two vacua by going through the saddle with energy E_{1a} [see Eq. (2.48)] is the domain wall. The one that goes through the saddle with energy $E_{1b}>E_{1a}$ is a wall-some sphaleron.

some sphaleron, i.e., a metastable configuration interpolating between the two vacua, which relaxes into the domain wall if subject to perturbations.[6]

In the limit $m\Sigma\ll\tau$, $\varphi_{II,III}\ll 1$, and the domain wall profile is essentially along the α direction. To estimate the tension of the domain wall, we first integrate out φ using Eq. (2.29)

$$\varphi\approx-\frac{m\Sigma}{2\tau}\cos\alpha \tag{2.34}$$

and substituting in Eq. (2.27) to get the potential energy for α:

[6]We thank A. Smilga for making this point clear to us. Wall-some sphalerons have been first discussed in the context of supersymmetric effective theories [25].

$$E(\alpha)=-\frac{m^2\Sigma^2}{2\tau}\cos^2\alpha. \tag{2.35}$$

We can then compute the tension of the domain wall as in the previous section, to get

$$\sigma_\alpha\approx\frac{2m\Sigma f_\pi}{\sqrt{\tau}}. \tag{2.36}$$

The error made by neglecting the gradient of the η' condensate φ within the domain wall can be estimated using Eq. (2.34) to eliminate α instead. This gives

$$\sigma_\varphi\approx\frac{\pi m^2\Sigma^2 f_\pi}{4\tau^{3/2}}, \tag{2.37}$$

which confirms that $\sigma_\varphi\ll\sigma_\alpha$ for $m\Sigma\ll\tau$.

How do these results compare to the predictions of chiral perturbation theory χPT? At leading order the potential vanishes at $\theta=\pi$. As discussed above, this corresponds to the limit $\tau\to\infty$ or $m_{\eta'}\to\infty$. Obviously, there is no trace of an η' condensate. As shown by Smilga, at next-to-leading order the only $\mathcal{O}(p^4)$ operator relevant at $\theta=\pi$ is O_7 (following the nomenclature of Gasser and Leutwyler [23]). Adding O_7 to Eq. (2.30) gives

$$E(\alpha)=-2m\Sigma\cos\frac{\theta}{2}\cos\alpha-4l_7\left(\frac{m\Sigma}{f_\pi^2}\right)^2\sin^2\frac{\theta}{2}\cos^2\alpha \tag{2.38}$$

or, at $\theta=\pi$,

$$E(\alpha)=-4l_7\left(\frac{m\Sigma}{f_\pi^2}\right)^2\cos^2\alpha. \tag{2.39}$$

Furthermore, in the large N_c limit, the η' is ''not that heavy'' $m_{\eta'}^2\sim 1/N_c$, and the coupling l_7 can be saturated by η' meson exchange [23],

$$l_7=\frac{f_\pi^2}{2m_{\eta'}^2}=\frac{f_\pi^4}{8\tau}, \tag{2.40}$$

where we used the Veneziano-Witten relation (2.4).[7] Substituting Eq. (2.40) in Eq. (2.39) gives back the large N_c prediction (2.35). Also, Eq. (2.36) reads

[7]In $SU(2)\times SU(2)$ chiral perturbation theory at finite N_c and finite strange quark mass, l_7 is instead saturated by η meson exchange, $l_7\propto 1/m_\eta^2\sim 1/m_s$. Although we have not pursued in this direction, most presumably the results of next-to-leading order $SU(2)\times SU(2)$ chiral perturbation theory could be recovered starting from the $SU(3)\times SU(3)$ case to leading order, and decoupling the strange quark. In the latter case, the vacuum degeneracy is indeed lifted already at leading order in χPT. Incidentally, this is precisely the reason why τ does not appear in the inequality (1.1). See the discussion of Smilga.

$$\sigma_\alpha \approx \frac{m\Sigma}{f_\pi}\sqrt{32 l_7}, \tag{2.41}$$

which is precisely the result derived by Smilga.

That predictions from next-to-leading order chiral χPT and the large N_c effective Lagrangian can be made to agree is a nice consistency check. As a bonus, in the large N_c framework, we see explicitly how the two degenerate vacua are related to spontaneous CP breaking with an η' condensate, and why they disappear as $\tau/m\Sigma\to\infty$, with a second order transition at $\theta=\pi$, features which, for obvious reasons, are not manifest within χPT.[8]

D. Two flavors, mass splitting effects

If $m_u\neq m_d$, the algebra is just a bit more cumbersome. Defining

$$z=m_d/m_u, \tag{2.42}$$

$$y=2\tau/\Sigma m_u, \tag{2.43}$$

and $\phi=\varphi+\pi/2$, the potential energy (2.5) at $\theta=\pi$ becomes

$$E=\Sigma m_u\{(1+z)\sin\varphi\cos\alpha+(1-z)\cos\varphi\sin\alpha+y\varphi^2\}. \tag{2.44}$$

In what follows, we will keep y fixed and vary z (i.e., m_d). Minimizing with respect to φ and α gives

$$\sin\alpha=-y\frac{1-z}{2z}\frac{\varphi}{\sin\varphi}, \tag{2.45}$$

while eliminating α, gives

$$\frac{\sin^2\varphi}{\varphi^2}\frac{4z^2}{y^2}=(1-z)^2+(1+z)^2\tan^2\varphi. \tag{2.46}$$

As for $z=1$, the CP conserving solution is again

$$\varphi_I=0,\quad \alpha_I=\pi/2\quad \text{modulo}\quad \pi. \tag{2.47}$$

Note however that, for $z\neq1$, these are two distinct solutions with energies

$$\begin{aligned} E_{Ia}&=(1-z)m_u\Sigma\equiv(m_u-m_d)\Sigma,\\ E_{Ib}&=-(1-z)m_u\Sigma\equiv(m_d-m_u)\Sigma. \end{aligned} \tag{2.48}$$

For $m_d>m_u$ (respectively $m_d<m_u$), E_{Ia} (E_{Ib}) has lower energy.

In the limit $m\Sigma\ll\tau$, we can write down the two CP violating solutions

$$|\varphi|\approx\frac{1}{1+z}\sqrt{4z^2/y^2-(1-z)^2}. \tag{2.49}$$

These exist provided

$$\left(\frac{2z^*}{y}\right)^2<(1-z_*)^2, \tag{2.50}$$

which gives two critical values of the mass ratio $z=m_d/m_u$,

$$z_1^*=\frac{y}{y+2}<1, \tag{2.51}$$

$$z_2^*=\frac{y}{y-2}>1. \tag{2.52}$$

For two light flavors, CP is spontaneously broken with a first order phase transition at $\theta=\pi$ if and only if[9]

$$z_1^*<\frac{m_d}{m_u}<z_2^*, \tag{2.53}$$

which is the equivalent for two flavors of Witten's inequality (1.1). For realistic quark mass and τ, Eq. (2.53) gives

$$\left|\frac{m_d-m_u}{m_u+m_d}\right|\lesssim\frac{m_\pi^2}{m_{\eta'}^2}, \tag{2.54}$$

which, just like Eq. (1.1), is unfortunately not satisfied in nature.[10]

For completeness, we give the CP violating solutions for z in the range of Eq. (2.53). Assuming small mass splitting, so that $\alpha\ll1$ modulo π, and using Eqs. (2.49) and (2.45), we have

$$\begin{aligned} &\varphi_{II}\approx-|\varphi|\quad\text{and}\quad \alpha_{II}\approx-\frac{y}{2z}(1-z),\\ &\varphi_{III}\approx|\varphi|\quad\text{and}\quad \alpha_{III}\approx\pi+\frac{y}{2z}(1-z). \end{aligned} \tag{2.55}$$

For larger mass splittings, CP violation goes away ($\varphi\to0$) and

$$\alpha_{II,III}\to-\frac{\pi}{2}\quad\text{mod}\quad\pi\quad\text{if}\quad z\to z_1^* \tag{2.56}$$

---

[8]As emphasized in [24], l_7 is anomalously large in the large N_c framework, $l_7=\mathcal{O}(N_c^2)$. If large N_c is adopted as a guideline, consistency would require to work with the extended symmetry $U(N_f)\times U(N_f)$, i.e. with a dynamical η', rather than $SU(N_f)\times SU(N_f)$. Our discussion provides another illustration of this point.

[9]That the two solutions z_1^* and z_2^* are not symmetric around $z=1$ is not surprising. At *fixed* m_u, the two limits, $z\to\infty$ and $z\to0$ correspond to two physically different situations: decoupling of a heavy quark in the former case ($N_f\to1$) and $N_f=2$ with a massless quark in the latter. The distinction goes however away for larger y's, $z^*\approx1\pm2/y$. If we exchange the role of m_d and m_u, $z\to z^{-1}$, $y\to zy$, and $z_1^*\leftrightarrow z_2^*$.

[10]Using the mass of π^0 and η', $\tau\sim(200\ \text{MeV})^4$ and $\Sigma\sim(250\ \text{MeV})^3$ (for $N_f=3$). As $m_u\approx4$ MeV and $m_d\approx7$ MeV, $y\sim40$ and $z_{1,2}^*\sim1\pm1/20$, to be compared to $m_d/m_u\approx1.75$.

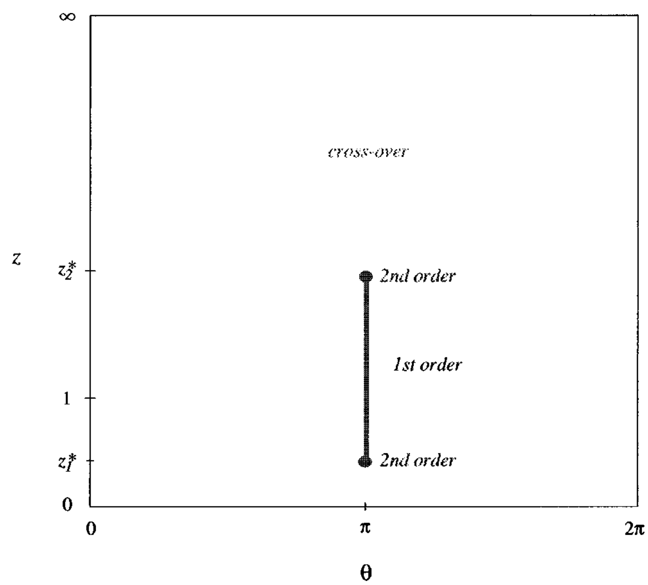

FIG. 4. Phase diagram of $N_f=2$ QCD in the $z-\theta$ plane, with $z=m_d/m_u$, for generic, *fixed* m_u and τ. Spontaneous CP violation occurs on the line of first order phase transitions at $\theta=\pi$ for $z_1^*<z<z_2^*$. Chiral perturbation theory at leading order corresponds to the particular limit in which $\tau\to\infty$ and $z_1^*=z_2^*=1$. If the quark mass increase for fixed τ, the critical line is stretched. In particular, $z_2^*\to\infty$ if $m_d\gg m_u$ ($N_f\sim 1$) and $m_u\gtrsim\tau/\Sigma$.

or

$$\alpha_{II,III}\to\frac{\pi}{2} \quad \text{mod} \quad \pi \quad \text{if} \quad z\to z_2^*. \tag{2.57}$$

The energy difference ΔE between the CP violating vacua and the *lowest energy* CP conserving saddle point of Eq. (2.48) is

$$\Delta E_{II}=\Delta E_{III}\approx-\frac{\Sigma^2 m_u^2}{2\tau}\left(\frac{z^*-z}{z^*-1}\right)^2, \tag{2.58}$$

which vanishes at $z=z_1^*$ or $z=z_2^*$. For $z\approx 1$, the tension of the domain wall relating the two CP violating vacua is well approximated by

$$\sigma\approx\frac{2m_u\Sigma f_\pi}{\sqrt{\tau}}\left|\frac{z^*-z}{z^*-1}\right|, \tag{2.59}$$

where, again, we are neglecting a small contribution from the η' condensate. [Compare with Eq. (2.36).] As z approaches $z_{1,2}^*$, the CP violating vacua merge into a unique, CP conserving vacuum and the domain wall disappears: the phase transition is of second order, with massless pion excitations. In particular, chiral perturbation theory at leading order corresponds to the limit $\tau\to\infty$, or $z_1^*=z_2^*=1$.

As can be seen on Fig. 3, for $z\neq 1$ there are apparently two distinct potential barriers between the two CP violating vacua, which correspond to the two CP conserving saddle points of Eq. (2.48). The configuration that relates the two vacua by going through the saddle point of higher energy at $\phi=0$ and $\alpha=\pi/2$ modulo π (2.48) is not a domain wall but a wall-some sphaleron, i.e., a metastable configuration which, if subject to the slightest perturbation, will relax to the domain wall configuration. This sphaleron is a remnant of the infinite family of equivalent domain walls that exist in the degenerate limit $m_u=m_d$. Similar objects have been encountered in supersymmetric theories [25].

III. SUMMARY: PHASE DIAGRAM OF QCD IN THE $z-\theta$ PLANE

For $N_f=2$, we have shown that CP is spontaneously broken at $\theta=\pi$ also for finite quark mass splitting, and derived the inequality (2.53), valid in the limit $m\Sigma\ll\tau$ ($m_\pi^2\ll m_{\eta'}^2$). The resulting phase diagram of $N_f=2$ QCD in the $z-\theta$ plane, where m_u and τ are held fixed and m_d is allowed to vary, is shown on Fig. 4. At $\theta=\pi$ there is a line of first order transitions for $z_1^*<m_d/m_u<z_2^*$. At the critical points z^*, the phase transition becomes of second order, while beyond these, there is just a smooth crossover. If the ratio $y=\tau/2m_u\Sigma$ increases, the critical lines shrinks to a point at $z^*=1$, with a second order phase transition. This is the limit described by leading order χPT. In the opposite limit of $m_u\Sigma\gtrsim\tau$, like at very large N_c or for heavy quarks, the critical line is stretched. If m_d decreases, spontaneous CP violation still goes away at some $0<z_1^*<1$. If m_d increases instead, the ''down quark'' eventually decouples and the system is essentially that of one flavor, $N_f=1$. In this case, if $m_u\Sigma\gtrsim\tau$, there is spontaneous CP violation at $\theta=\pi$ for any m_d and z_2^* goes to infinity. Finally, if both quarks are heavy, the system is analogous to pure Yang-Mills theory, and CP is always broken at $\theta=\pi$. This completes our survey of Dashen's phenomenon for $N_f=0,1,2$.

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