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CP-violating theta parameter in the domain model of the QCD vacuum

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A nonzero CP -violating θ parameter is treated in the domain model which assumes a clusterlike vacuum structure whose units are characterized, in particular, by a topological charge which is not necessarily an integer number. In the present paper we restrict consideration to rational values of the charge. The model has previously been shown to manifest confinement, spontaneous chiral symmetry breaking and the absence of an axial $U(1)$ Goldstone boson. We find that the specific structure of the minima of the free energy density of the domain ensemble forces a 2π periodicity of observables in θ for any number of light quarks, that vacuum doubling occurs at $\theta = \pi$ for any $N_f > 1$ and any value of topological charge q . These features are in agreement with expectations based on anomalous Ward identities and large N_c effective theories. We find also additional values of θ depending on q for which vacuum doubling occurs.

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I. INTRODUCTION

Explicit CP violation can be introduced in quantum chromodynamics by the inclusion of the so-called theta term in the action. In Euclidean space this amounts to

$$S_\theta = iq\theta, \quad q = \frac{g^2}{32\pi^2} \int d^4x F_{\mu\nu} \tilde{F}^{\mu\nu}. \quad (1)$$

A remarkable feature of such a term in the presence of spontaneously broken chiral symmetry is the Dashen phenomenon [1]: this explicit breaking of CP can become spontaneous due to vacuum doubling at the point $\theta = \pi$. This value falls outside the physically relevant range $0 \leq \theta \leq 10^{-9}$ to which θ is constrained by the neutron dipole moment [2] and current algebra [3]. Nonetheless, the Dashen phenomenon is a constraint on self-consistent models of the nonperturbative QCD vacuum. The statement of the problem related to the Dashen phenomenon as well as the question about periodic dependence of observables in θ acquires full sense only if the values of q are not restricted to integers. In this paper we use the domain model [4] of the QCD vacuum to show how specific properties of quark field configurations summed up in the partition function can lead to the periodic dependence on θ and to the Dashen phenomenon for any rational values of q .

The approaches which originally demonstrated the Dashen phenomenon in the context of QCD are those of anomalous Ward identities [5] and effective chiral Lagrangians [6] in the limit of a large number of colors N_c , which we shall describe below in more detail. Subsequent discussions of the Dashen phenomenon include [7–11]. This phenomenon for $\theta \neq 0$ is intimately

related to both the mechanism of spontaneous chiral symmetry breaking and the nonappearance of an axial $U(1)$ pseudoscalar Goldstone boson as shown by the original works revealing it in QCD. In [5] the key tool is the generalization to the axial $U(1)$ channel of Ward identities in which the true vacuum of the theory is unknown, but for which divergences of current-current expectation values in this vacuum can be related to hadron spectroscopy via vacuum symmetry properties. For example, the light pion mass as input into the flavor $SU(2)_L \times SU(2)_R$ Ward identity (which gives the Gell-Mann–Oakes–Renner relation) leads to a nonzero chiral condensate as the output. In the axial $U(1)$ channel (where the anomaly figures) and $\theta = 0$ the phenomenological input is now the absence of a light meson, with the output that topological charge q must be fractional. With $\theta \neq 0$ the corresponding output starting with the same phenomenological input is 2π periodicity in θ and the property of vacuum doubling and spontaneous CP breaking at $\theta = \pi$. In the large N_c approach the same data are turned around. An effective Lagrangian for mesons is written down for $N_c \rightarrow \infty$ which assumes chiral symmetry breaking and the anomaly. The output for $\theta = 0$ includes the famous relation between the topological susceptibility and various meson masses. For $\theta \neq 0$ again the Dashen phenomenon emerges.

However these approaches do not unveil the actual mechanism of nonperturbative vacuum properties such as confinement and spontaneous chiral symmetry breaking. The domain model [4] is a bottom up approach to these features: a particular vacuum structure is introduced into the formalism explicitly, here based on a statistical ensemble of domainlike gluon fields, and out of this both vacuum and mesonic properties are derived. In previous works both confinement [4] and chiral symmetry realization [12,13] have been studied for this vacuum *ansatz*. The

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anomaly contribution to the free energy suppresses continuous axial $U(1)$ degeneracy in the ground state, leaving only a discrete residual axial symmetry. This discrete symmetry and flavor $SU(N_f)_L \times SU(N_f)_R$ chiral symmetry in turn are spontaneously broken with a quark condensate arising due to the asymmetry of the spectrum of the Dirac operator in the domain background. An estimate of pseudoscalar and vector meson masses has been computed showing the typical pattern of spontaneous breakdown of $SU(N_f)_L \times SU(N_f)_R$ chiral symmetry with the correct splitting between π , η and η' mesons [13]. In this paper we test the model against the above predictions of spontaneous CP breaking and generally explore its features for the nonzero θ parameter. The Dashen phenomenon is studied by directly computing the θ dependence of the free energy density and chiral condensate within the domain model.

The results of this paper are that indeed the vacuum doubling at $\theta = \pi$ occurs in the domain model for any rational values of the topological charge q and any number of flavors. Thus the domain model provides an explicit example of simultaneous realization of confinement and chiral symmetry breaking where the Dashen phenomenon is manifest. Within the model, the topological charge is not restricted to any *ad hoc* value, and in the general case there are critical values in addition to $\theta = \pi$, which disappear when q is set to $1/N_f$ (which is the value of q emerging in [5] for the case of N_f degenerate quark flavors). In particular, in [4] the domain model parameters were fixed from the string tension giving $q = 0.15$. For this topological charge, the critical values $\theta = -\pi/3, \pi/3, \pi(\text{mod } 2\pi)$ appear for which the vacuum doubling occurs. As with [5], vacuum degeneracy for discrete θ and 2π periodicity of observables such as the condensate arises as output rather than being assumed. Unlike [5,6], these results emerge without the absence of a massless $U(1)$ boson being input.

We first briefly review the domain model for $\theta = 0$ and thereafter examine the realization of chiral symmetry for $\theta \neq 0$. In the Appendixes we review and compare our results with the approaches of [5,6].

II. REVIEW OF CHIRAL SYMMETRY IN THE DOMAIN MODEL

For motivation and a detailed description of the domain model we refer the reader to [4]. The essential definition of the model is given in terms of the following partition function for $N \rightarrow \infty$ domains of radius R :

$$\begin{aligned} Z = & \mathcal{N} \lim_{V, N \rightarrow \infty} \int_{-\infty}^{\infty} d\alpha \prod_{i=1}^N \int_{\Sigma} d\sigma_i \int_{\mathcal{F}_{\psi}^i} \mathcal{D}\psi^{(i)} \mathcal{D}\bar{\psi}^{(i)} \\ & \times \int_{\mathcal{F}_Q^i} \mathcal{D}Q^i \delta[D(\check{B}^{(i)})Q^{(i)}] \Delta_{\text{FP}}[\check{B}^{(i)}, Q^{(i)}] \\ & \times e^{-S_{V_i}^{\text{QCD}}[Q^{(i)+B^{(i)}, \psi^{(i)}, \bar{\psi}^{(i)}]} \end{aligned} \quad (2)$$

where the functional spaces of integration \mathcal{F}_Q^i and \mathcal{F}_{ψ}^i are specified by the boundary conditions $(x - z_i)^2 = R^2$

$$\begin{aligned} \check{n}_i Q^{(i)}(x) = 0, \quad i \check{\eta}_i(x) e^{i\alpha\gamma_5} \psi^{(i)}(x) = \psi^{(i)}(x), \\ \bar{\psi}^{(i)} e^{i\alpha\gamma_5} i \check{\eta}_i(x) = -\bar{\psi}^{(i)}(x). \end{aligned} \quad (3)$$

Here $\check{n}_i = n_i^a t^a$ with the generators t^a of $SU_c(3)$ in the adjoint representation and α is a random chiral angle associated with the chiral symmetry violating boundary condition Eq. (3) in the presence of one species of quark. The generalization to N_f flavors is given in the next section. The thermodynamic limit assumes $V, N \rightarrow \infty$ but with the density $\nu^{-1} = N/V$ taken fixed and finite. The partition function is formulated in a background field gauge with respect to the domain mean field, which is approximated inside and on the boundaries of the domains by a covariantly constant (anti-)self-dual gluon field with the field-strength tensor of the form

$$F_{\mu\nu}^a(x) = \sum_{j=1}^N n^{(j)a} B_{\mu\nu}^{(j)} \vartheta[1 - (x - z_j)^2/R^2],$$

with $B_{\mu\nu}^{(j)} B_{\mu\rho}^{(j)} = B^2 \delta_{\nu\rho}$. Here z_j^μ are the positions of the centers of domains in Euclidean space.

In order to reflect continuity of colorless quark currents at the positions of pure gauge singularities in the picture of quark and gluon configurations, which is approximated by the domain model, the chiral angle α is taken to be the same for all domains in the representation Eq. (2). This is a refinement of the formulation presented in [4,12,13]. The measure of integration over parameters characterizing domains is

$$\begin{aligned} \int_{\Sigma} d\sigma_i \cdots = & \frac{1}{48\pi} \int_V \frac{d^4 z_i}{V} \int_0^{2\pi} d\varphi_i \int_0^\pi d\vartheta_i \sin\theta_i \\ & \times \int_0^{2\pi} d\xi_i \sum_{l=0,1,2}^{3,4,5} \delta\left(\xi_i - \frac{(2l+1)\pi}{6}\right) \\ & \times \int_0^\pi d\omega_i \sum_{k=0,1} \delta(\omega_i - \pi k) \cdots, \end{aligned} \quad (4)$$

where (θ_i, φ_i) are the spherical angles of the chromomagnetic field, ω_i is the angle between chromoelectric and chromomagnetic fields and ξ_i is an angle parametrizing the color orientation.

This partition function describes a statistical system of domainlike structures of density ν^{-1} , where the volume of a domain is $\nu = \pi^2 R^4/2$. Each domain is characterized by a set of internal parameters and with internal dynamics represented by fluctuation gluon $Q^{(i)}$ and quark $\psi^{(i)}$ fields. It respects the symmetries of the QCD Lagrangian, since the statistical ensemble is invariant under space-time, color gauge and particularly chiral symmetries. Thus the model involves two free parameters: the mean field strength B and the mean domain radius R . These dimensionful parameters break the scale invariance present originally in the QCD

Lagrangian. In principle, they should be related to the trace anomaly of the energy-momentum tensor [14,15] and, eventually, to the fundamental scale Λ_{QCD} . Knowledge of the full quantum effective action of QCD would be required for establishing a relation of this kind. Within this framework the gluon condensate to lowest order in fluctuations is $4B^2$ and the topological charge per domain is $q = B^2 R^4 / 16$.

An area law is obtained for static quarks. The reason for this is the finite range of gluon correlations implicit in the model which will figure in all the phenomena we consider. Computation of the Wilson loop for a circular contour of a large radius $L \gg R$ gives a string tension $\sigma = Bf(\pi BR^2)$ where f is given for color $SU(2)$ and $SU(3)$ in [4]. Estimations of the values of these quantities are known from lattice calculation or phenomenological approaches and can be used to fit B and R . As described in [4] these parameters are fixed to be $\sqrt{B} = 947 \text{ MeV}$, $R = (760 \text{ MeV})^{-1} = 0.26 \text{ fm}$ with the average absolute value of topological charge per domain turning out to be $q = 0.15$ and the density of domains $\nu^{-1} = 42 \text{ fm}^{-4}$. The topological susceptibility then turns out to be $\chi = (197 \text{ MeV})^4$, comparable to the Witten-Veneziano value [6]. The eigenvalue problem

$$\not{D}\psi(x) = \lambda\psi(x), \quad (5)$$

with boundary condition Eq. (3) was studied in [12]. With the domain background field the solution to this problem reveals an asymmetric spectrum, exhibiting the broken chiral symmetry through the baglike boundary condition, and thus none of the eigenmodes is chiral. However at the center of domains all modes are chiral and the sign of their chirality depends on whether the underlying gauge field is self-dual or anti-self-dual. In [12] we computed the distribution of values of the local chirality parameter of [16] in a chirally symmetric ensemble revealing qualitatively similar behavior to the double-peak structure seen on the lattice [17], which is taken to be indicative of spontaneously broken chiral symmetry.

The α -dependent part of the free energy density was computed in [13] using zeta function regularization, with an imaginary part arising

$$\text{Im}F = \pm \frac{q}{\nu} \arctan[\tan(\alpha)] \quad (6)$$

where q is the absolute value of topological charge in a domain, and overall sign $(-)+$ corresponds to an (anti-)self-dual domain. The charge is not integer here in general but the anomalous term is nonetheless πn periodic in α . This is the Abelian anomaly as observed within the context of baglike boundary conditions by [18] and is consistent with [19] albeit not generated from purely chiral zero modes but the chiral properties of nonzero modes.

The part of the free energy density \mathcal{F} relevant for the present consideration of an ensemble of $N \rightarrow \infty$ domains with both self-dual and anti-self-dual configurations takes

the form

$$\begin{aligned} e^{-\nu N \mathcal{F}} &= \mathcal{N} \int_{-\infty}^{\infty} d\alpha [\cos \nu \text{Im}F(\alpha)]^N \\ &= \mathcal{N} \sum_{\alpha \in \alpha_{\min}} \exp(N \ln[\cos(\nu \text{Im}F(\alpha))]) + O(1/N). \end{aligned}$$

Here the summation goes over the infinite set α_{\min} of degenerate minima of the free energy density, which are achieved at

$$\nu \text{Im}F(\alpha_{\min}) = 0 \pmod{2\pi}.$$

In the thermodynamic limit $N \rightarrow \infty$ the solutions to the above equation for α_{\min} correspond to a degenerate set of vacua connected by discrete chiral transformations, which will be given in the next section.

Thus for massless quarks, a discrete subgroup of $U_A(1)$, rather than the continuous $U_A(1)$ itself, represents a symmetry of the vacua. The anomaly defines those chiral angles which minimize the free energy so that the full $U_A(1)$ group is no longer reflected in the vacuum degeneracy. It should be stressed here that this residual discrete degeneracy ensures a zero value for the quark condensate in the absence of mass term or some other external chirality violating sources.

In the presence of an infinitesimally small quark mass the α dependent part of the free energy of a self-dual domain is modified by the term linear in mass and takes the form (for details see [13])

$$\begin{aligned} F &= i \frac{q}{\nu} \arctan[\tan(\alpha)] - m \varkappa e^{i\alpha} + O(m^2), \\ \varkappa &= \frac{1}{\pi^2 R^3} \sum_{k=1, z=z_1, z_1, z_2}^{\infty} \frac{k}{k+1} \left[M(1, k+2, z) \right. \\ &\quad \left. - \frac{z}{k+2} M(1, k+3, -z) - 1 \right], \end{aligned} \quad (7)$$

where the quantity $\varkappa > 0$ comes from the spectral asymmetry term $\eta(1)$,

$$\eta(s) = \sum_{\lambda} \text{sgn}(\lambda) / |\lambda|^s,$$

appearing due to the asymmetry of the spectrum [20]. The free energy of an anti-self-dual domain is obtained via complex conjugation.

This discrete chiral symmetry of the massless case is spontaneously broken and switching on the quark mass selects one of the vacua. For our conventions of boundary condition and mass term the selected minimum is at $\alpha = 0$. It is important that values for the angles α_{\min} are not modified by the leading order term, linear in m . The quark condensate is extracted from the free energy in the standard way

$$\langle \bar{\psi}(x)\psi(x) \rangle = -\lim_{m \rightarrow 0} \lim_{N \rightarrow \infty} \frac{1}{\nu N} \frac{d}{dm} e^{-\nu N \mathcal{F}(m)} = -\varkappa \quad (8)$$

and takes the value $\langle \bar{\psi}(x)\psi(x) \rangle = -(237.8 \text{ MeV})^3$ for the

values of field-strength B and domain radius R fixed earlier by consideration of the pure gluonic characteristics of the vacuum—string tension, topological susceptibility and gluon condensate.

For $N_f > 1$ quark flavors the fermion boundary condition in Eq. (3), explicitly breaks all chiral symmetries, flavor singlet and nonsinglet (see also [18]). Thus integrating over all α does not suffice to provide for the full chiral invariance of the ensemble of quark configurations contributing to the partition function. Rather, the boundary condition must be generalized to include flavor nonsinglet angles, $\alpha \rightarrow \alpha + \beta^a T^a/2$, with T^a the $N_f^2 - 1$ generators of $SU(N_f)$. Then integration over N_f^2 angles α and β^a must be performed for a fully chiral symmetric ensemble. The spectrum of the Dirac operator can be found now quite analogously to the one-flavor case, except that the boundary condition mixes flavor components and an additional projection into flavor sectors is required in order to solve Eq. (5). The calculation from this point will be repeated for nonzero θ in the next section, but it suffices to summarize here the result for $\theta = 0$ emerging in [13]: the Abelian nature of the anomaly meant that the nonsinglet chiral angles implicit in this procedure drop out of the ensemble free energy. Thus there are only $N_f^2 - 1$ continuous directions in the vacuum. The expectation that there should be only $N_f^2 - 1$ pseudo-Goldstone bosons has been verified in [13] for $N_f = 3$ by an estimation of the meson spectrum.

III. FREE ENERGY IN THE PRESENCE OF NONZERO θ

Now we include the CP -violating parameter in the model by the additional term Eq. (1) in the action, which contributes a pure phase to the weight factor in Euclidean space. Integrating over N_f fermions with infinitesimally small masses $m_1 = \dots = m_N \equiv m$ in a domain ensemble gives for the free energy density per domain

$$F = -v^{-1} \ln \cos q[W_{N_f} - \theta] - m\kappa \sum_{i=1}^{N_f} \cos \Phi_i, \quad (9)$$

where

$$W_{N_f} = \sum_{i=1}^{N_f} \arctan(\tan \Phi_i), \quad (10)$$

$$\Phi_i = \alpha + B_i, \quad B_1 = 0, \quad \text{for } N_f = 1, \quad (11)$$

$$B_1 = \frac{|\vec{\beta}|}{2}, \quad B_2 = -\frac{|\vec{\beta}|}{2}, \quad \text{for } N_f = 2, \quad (12)$$

and

$$\begin{aligned} B_1 &= b^3 + b^8/\sqrt{3}, & B_2 &= -b^3 + b^8/\sqrt{3}, \\ B_3 &= -2b^8/\sqrt{3}, & & \text{for } N_f = 3. \end{aligned} \quad (13)$$

Here α is the $U(1)$ chiral angle, $\vec{\beta}$ are the nonsinglet chiral angles for $N_f = 2$, and b_3 and b_8 are certain functions of the eight nonsinglet chiral angles β^a for $N_f = 3$. For $N_f = 1$, Eq. (11) is just the result discussed in the previous section. For $N_f = 2$ the quantities B_1 and B_2 in Eq. (12) arise from the projection of the quark boundary condition into $SU(2)$ flavor sectors. For $N_f > 2$ the analogous functions are B_1, \dots, B_{N_f} . For any number of flavors N_f the functions B_i have the property that

$$\sum_{i=1}^{N_f} B_i = 0 \quad (14)$$

which manifests the tracelessness of the flavor generators in any basis. Thus

$$\sum_{i=1}^{N_f} \Phi_i = N_f \alpha. \quad (15)$$

The ‘‘arctantan’’ structure in Eq. (10) manifests the periodicity of the free energy for arbitrary topological charge q . We could write

$$W_{N_f} = \sum_{i=1}^N \arctan[\tan \Phi_i] = N_f \alpha \pmod{\pi} \quad (16)$$

which is independent of the β^a . This is the Abelian property of the anomaly leading to the expectation of $N_f^2 - 1$ Goldstone bosons.

The central effect is the chiral Abelian anomaly contribution denoted as qW_{N_f} under the cosine in Eq. (9). It should be noted that

$$qW_{N_f} = N_f q \alpha + O(\alpha^2) \quad \text{for } \alpha \rightarrow 0, \quad (17)$$

which coincides with the standard form of axial anomaly in the Fujikawa derivation (note that α here is twice the angle of chiral transformation used in Fujikawa’s calculation of anomaly [19]).

The mass term is introduced as a small perturbation violating explicitly the chiral symmetry of the system. In the absence of the mass term, the minima of the free energy are determined by the solutions

$$\alpha_{kl}(\theta) = \frac{\theta}{N_f} + \frac{2\pi l}{qN_f} + \frac{\pi k}{N_f} \quad (k \in \mathbb{Z}, l \in \mathbb{Z}), \quad (18)$$

to the equation

$$\cos(qW_{N_f} - q\theta) = 1. \quad (19)$$

Evidently there are multiple solutions arising from the various periodic functions appearing in Eq. (9). The index k in the solutions reflects periodicity of \tan while l corresponds to the periodicity of \cos in Eq. (19). Note that these solutions do not depend on the flavor nonsinglet chiral angles, as discussed above, and thus the free energy displays continuous degeneracy with respect to these angles.

The solutions Eq. (18) give an infinite discrete set of degenerate minima of the free energy density. For given N_f and q a finite subset of these minima can be extracted such that all other minima are 2π -periodic copies of one of the already identified vacua. For instance, for $N_f = 1$ and $q = 0.15$ the six different vacua correspond to all combinations of $k = 0, 1$ and $l = 0, 1, 2$, while for $N_f = 2$ set of “different” minima is given by combinations of $k = 0, 1, 2, 3$ and $l = 0, 1, 2$. It is clear that the system of minima is 2π periodic with respect to θ :

$$\alpha_{kl}(\theta + 2\pi m) \rightarrow \alpha_{k'l}(\theta), \quad k' = k + 2m, \quad (20)$$

and the shift in θ can be undone by reenumerating the infinite set of minima. This periodicity does not depend on the value of q at all since it is ensured by reenumerating of index k without use of l . All minima are degenerate (the free energy is equal to zero) for zero quark mass.

Switching on the infinitesimal mass term in Eq. (9) lifts the degeneracy due to different values of the symmetry breaking term

$$V_m = -m\kappa \sum_i^{N_f} \cos\Phi_i^{kl}(\theta) \quad (21)$$

in the free energy for different $\Phi_i^{kl} = \alpha_{kl}(\theta) + B_i(\beta^a)$. This introduces nonsinglet angle dependence into the free energy, which must now also be minimized with respect to the β^a . To this end we expand V_m in small fluctuations in the B_i and look for minima, bearing in mind the constraint Eq. (14). The condition that V_m have stationary points leads to the condition

$$\sin\Phi_i \text{ independent of } i \quad (22)$$

while the condition that this leads to a minimum forces

$$\cos\Phi_i > 0. \quad (23)$$

Equation (22) leads to $\Phi_i = \alpha + B_i$ being independent of i which means $B_i = 0(\text{mod } 2\pi)$. On the other hand, Eq. (23) is fulfilled by restricting $-\pi/2 \leq \Phi_i(\text{mod } 2\pi) \leq \pi/2$. However, we observe that for these values of Φ_i

$$\arctan[\tan\Phi_i] = \Phi_i(\text{mod } 2\pi).$$

Thus to guarantee a minimum with respect to nonsinglet angles, we must have

$$W_{N_f} = \sum_{i=1}^{N_f} \arctan[\tan\Phi_i] = N_f \alpha(\text{mod } 2\pi).$$

Comparing to Eq. (16), we see that of the vacua of the massless free energy, $\alpha_{kl}(\theta)$, only those with k an *even* integer correspond to true minima with the mass term switched on. Note that these arguments only apply for $N_f > 1$. For the single flavor case the available values are $k = 0, 1$. A similar consideration shows that for rational $q = n_1/n_2$ the minima selected by the mass term correspond to l any integer if n_1 is odd but l even if n_1 is even.

The result is that the θ dependence of the quark condensate is given by

$$\langle \bar{\psi}(x)\psi(x) \rangle_{\alpha_{kl}(\theta)} = -N_f \kappa \cos\alpha_{kl}(\theta)$$

for k even and l any integer except if $q = n_1/n_2$ with n_1 even for which then l is also even. This is plotted in Figs. 1 and 2 for $N_f = 1$ and $N_f = 3$ respectively, where the cosine in Eq. (21) is plotted as a function of θ for the minima which are not 2π equivalent. Critical values of θ correspond to the points where two minima become degenerate.

The two degenerate vacua at such critical points are distinguished by their *CP* properties, which can be seen from the behavior of the pseudoscalar condensate as a function of θ

$$\langle \bar{\psi}(x)\gamma_5\psi(x) \rangle_{\alpha_{kl}(\theta)} = -N_f \kappa \sin\alpha_{kl}(\theta),$$

as derived for the domain model in Appendix A. As expected, the scalar [see Eq. (21)] and pseudoscalar condensates depend on θ through cosine and sine of $\alpha_{kl}(\theta)$ respectively.

The plots for one and three flavors, respectively, are given in Figs. 3 and 4 again with $q = 0.15$. The pseudoscalar condensate is discontinuous at the critical values of θ and takes values opposite in sign for the two degenerate minima: parity is thus spontaneously broken.

In other words, we can see that for most values of theta the mass term selects a unique minimum of the free energy. However, there are critical values of θ where two different minima are degenerate, thus displaying a twofold degeneracy of the vacuum in the presence of a mass.

There are two conditions for critical θ . The first one is obviously

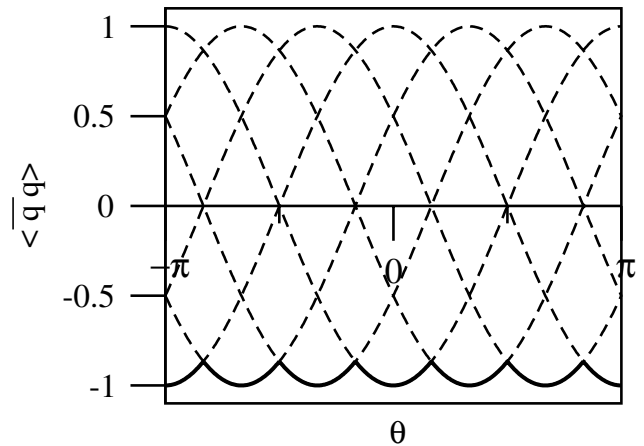


FIG. 1. The scalar quark condensate as a function of the parameter θ for $N_f = 1$ and $q = 0.15$ in units of κ . The dashed lines correspond to discrete minima of the free energy density which are degenerate for $m \equiv 0$. The solid line denotes the minimum which becomes global for a given θ in the presence of an infinitesimally small mass term.

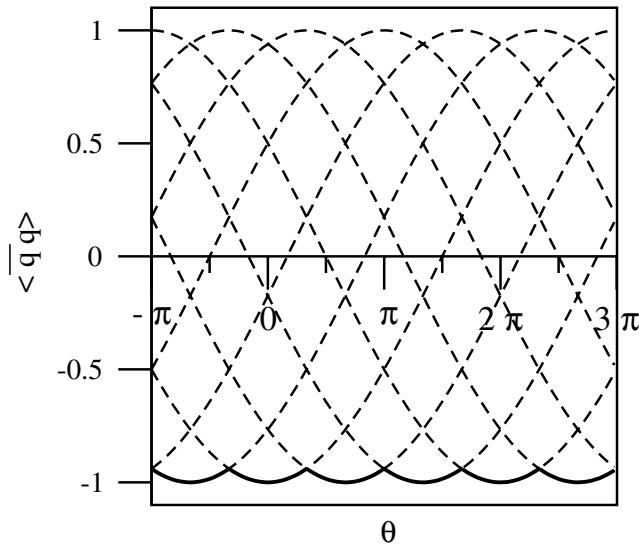


FIG. 2. The scalar quark condensate as a function of θ for $N_f = 3$ and $q = 0.15$ in units of \aleph . The meaning of dashed and solid lines is the same as in Fig. 1. Qualitatively the picture is the same as for $N_f = 1$: the same periodicity and critical values of θ , which is achieved by an increased number of different discrete minima.

$$\alpha_{00}(\theta_{\text{crit}}) = -\alpha_{kl}(\theta_{\text{crit}})(\text{mod } 2\pi)$$

where k and l should not be equal to zero simultaneously and without loss of generality we have taken α_{00} on the right-hand side. Thus

$$\theta_{\text{crit}}^{kl} = \pi k + \frac{l\pi}{q}(\text{mod } 2\pi).$$

For a given q this defines a set of values of $\theta_{\text{crit}}^{kl}$ where several vacua are degenerate. This set is independent of a number of flavors N_f . Furthermore, we are interested only

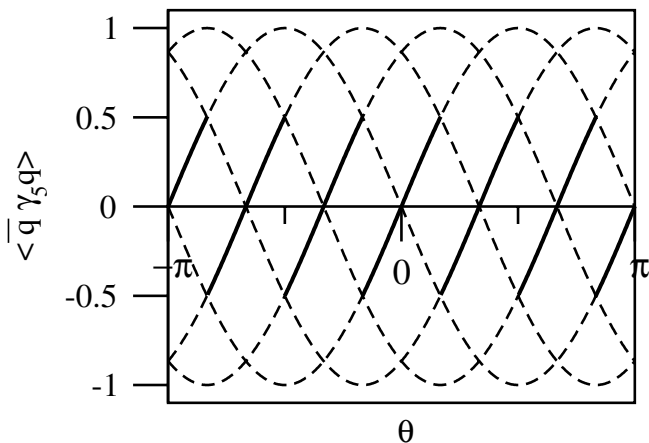


FIG. 3. The pseudoscalar quark condensate as a function of θ for $N_f = 1$ and $q = 0.15$ in units of \aleph . The meaning of dashed and solid lines is the same as in Fig. 1.

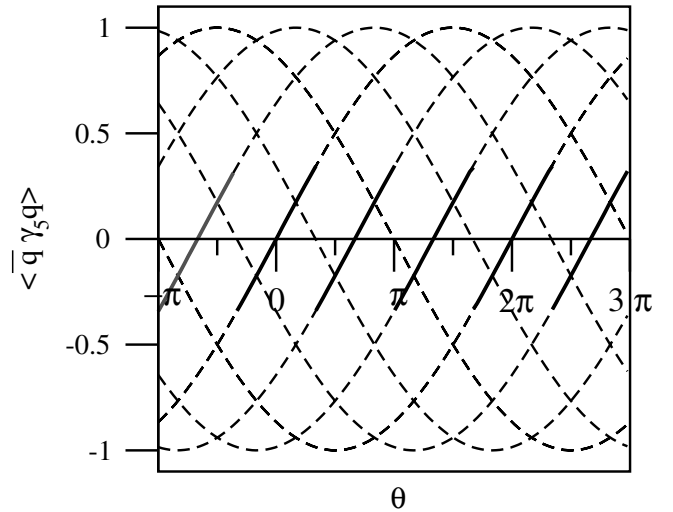


FIG. 4. The pseudoscalar quark condensate as a function of θ for $N_f = 3$ and $q = 0.15$ in units of \aleph . The meaning of dashed and solid lines is the same as in Fig. 2.

in those $\theta_{\text{crit}}^{kl}$ which minimize the term linear in mass, which is the second condition for θ_{crit} . It is easy to check that independently of q the value $\theta_{\text{crit}} = \pi$ satisfies both conditions. Other critical values depend on topological charge of the domain q . In general if $q = n_1/n_2$ then there are n_1 critical values of theta. For the value $q = 0.15$, as was fit in the domain model, we find

$$\theta_{\text{crit}} = \{-\pi/3, \pi/3, \pi\}(\text{mod } 2\pi),$$

where the Dashen phenomenon occurs. We conclude that for any N_f and rational q there is a finite number of critical points in the interval $[0, 2\pi]$ including $\theta = \pi$.

IV. SUMMARY AND DISCUSSION

The central result of this paper is that 2π periodicity of amplitudes in θ and vacuum doubling with spontaneous CP violation at certain critical values of θ , in particular $\theta = \pi$, are obtained for any number of light flavors N_f and arbitrary rational topological charge q . This is achieved in a model whose input is a particular class of nonperturbative gluon configurations. From this model have been derived both confinement, the correct pattern of chiral symmetry breaking, certain static characteristics of the vacuum (string constant, condensates, topological susceptibility) as well as properties of the meson spectrum (correct splitting between masses of isovector and isosinglet states). The most important qualitative feature of this class of vacuum fields is that it can be seen as an ensemble of densely packed lumps of (anti-)self-dual gluon fields, characterized by a finite correlation length. In this paper and in previous works it has been shown on a semiquantitative level that such vacuum fields can reproduce all of the qualitatively

important features of the QCD vacuum associated with confinement and chiral symmetry realization.

We discuss now our results in light of the two main approaches, that of anomalous Ward identities and of the effective chiral Lagrangian at large N_c , which originally predicted the Dashen phenomenon in the presence of a theta term. For convenience, we have summarized the salient features of these approaches in Appendix B.

The first point of comparison is the minimization with respect to nonsinglet angles. In both [5,6], this is referred to as ‘‘Dashen’s theorem.’’ In the domain model context, precisely the same conditions Eqs. (22) and (23) have arisen by considering the free energy as a function of the dynamical variables β^a associated with the flavor nonsinglet angle dependence of fermion boundary conditions. In [5,6] the corresponding angles are denoted ϕ_i corresponding to the phases of an $N_f \times N_f$ matrix, either the matrix of scalar condensates $\langle \bar{\psi}_i \psi_j \rangle$ in [5] or the chiral field of [6]. In all cases, these results (for the degenerate mass case) emerge because of the structure of the symmetry breaking term $-m\aleph \sum_{i=1}^{N_f} \cos \Phi_i$. The significance of this structure for the domain model is that it emerges precisely from the spectral asymmetry of the Dirac operator in the domain field background as computed via zeta function regularization [12]. The analogs of the ϕ_i in [5,6] are our functions Φ_i associated with the flavor dependence of the fermion domain boundary conditions.

The second point of contact relates to the existence or otherwise of an axial $U(1)$ Goldstone boson in the spectrum. In both [5,6], the *input* that there be no such boson leads to a constraint on the sum of the aforementioned angles ϕ_i and the theta parameter:

$$\sum_{i=1}^{N_f} \phi_i = \theta. \quad (24)$$

In the domain model approach, as mentioned at the outset, the anticipated absence of such a boson is a *consequence* of the lack of continuous axial $U(1)$ degeneracy of the ground state of the free energy for the massless case. But this ground state is determined by

$$\sum_{i=1}^{N_f} \arctan(\tan \Phi_i) = \theta \quad (25)$$

from Eq. (19). Resolving the arctantan structure brings us to the same form as in Eq. (24), when ϕ_i and Φ_i are identified, again consistent with our observations above.

Certainly the reason for these coincidences is most transparent in the comparison to the large N_c approach, reviewed in Appendix B: the effective singlet and nonsinglet meson fields there are contained in $U(N_f)$ matrices but diagonalized by $SU(N_f) \times SU(N_f)$ transformations. In the domain model, where the conditions on quark fields at domain boundaries also involve the $U(N_f)$ flavor matrices

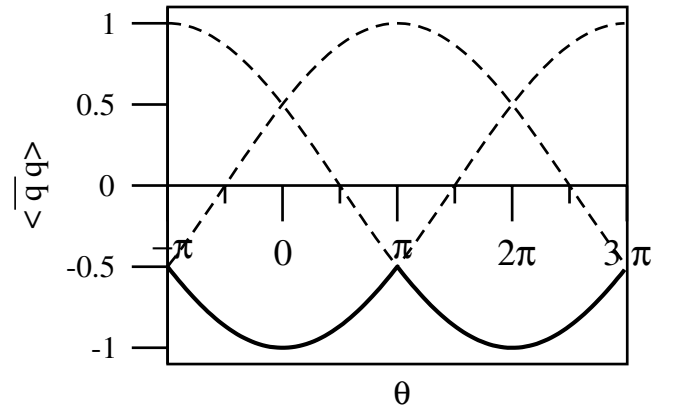


FIG. 5. The scalar quark condensate as a function of θ for $N_f = 3$ and $q = 1/N_f$ in units of \aleph , which is equivalent to a corresponding plot from [5]. The meaning of dashed and solid lines is the same as in Fig. 1.

$\exp[i(\alpha + \beta^a T^a/2)\gamma_5]$ which are similarly diagonalized by special unitary matrices.

The main difference with [5] is the specific value of the topological charge. For a more direct comparison with [5] we set $q = 1/N_f$ in our formula, Eq. (18). The l -dependent term is then $2\pi l$ which is inconsequential under the cosine for the condensate. Thus our results completely agree with [5] for this case. For the $N_f = 3$ case, we plot the scalar and pseudoscalar condensates in Figs. 5 and 6 which are identical to corresponding plots in [5].

The significance of our result in comparison to [5,6] is that the domain model assumes the dominance of a specific class of nonperturbative gluon configurations in the QCD functional integral and thereby provides the 2π periodicity in theta dependence and the existence of critical values of theta parameter as output simultaneous with the correct resolution of the axial $U(1)$ problem. In [5,6] the absence of a pseudoscalar $U(1)$ boson is input in order to obtain the

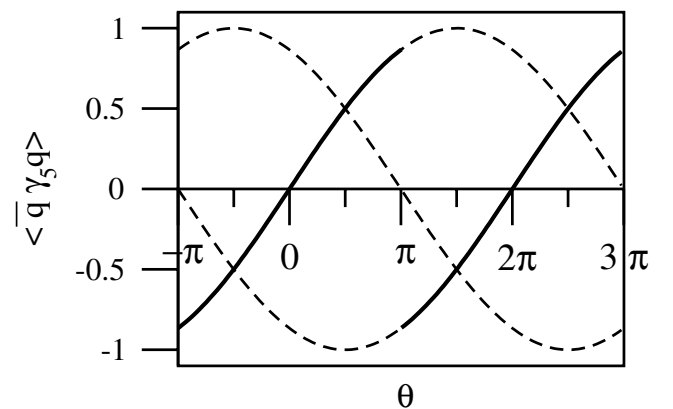


FIG. 6. The pseudoscalar quark condensate as a function of θ for $N_f = 3$ and $q = 1/N_f$ in units of \aleph . The meaning of dashed and solid lines is the same as in Fig. 1.

theta dependence, while the responsible vacuum structure is unknown.

The present work can be generalized for the case of nondegenerate quark masses in the presence of the theta term for which an analysis using anomalous Ward identities is given in [5]. Because of the above-noted similarities with the domain model the condensate dependence on θ will be identical.

Finally, we mention that the model under consideration with rational topological charges q reflects the strong CP problem in the usual way, but certainly cannot resolve it. As in several other approaches (for instance [21]) we notice that the free energy in the model is minimized by $\theta = 0$, but there is no reason within the model to demand the minimization of the free energy with respect to θ , which is an external parameter here. However, allowing irrational values of q can drastically change the status of the strong CP problem in the model due to the appearance of infinitely many critical values of θ in any finite interval. We shall analyze this intriguing possibility in a separate publication.

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APPENDIX A: PSEUDOSCALAR CONDENSATE

We treat here $N_f = 1$ and the integral for one domain for simplicity; the generalization is straightforward. Consider

$$\langle \bar{\psi} e^{i\beta\gamma_5} \psi \rangle_\alpha = \frac{1}{2} [\langle \bar{\psi} e^{i\beta\gamma_5} \psi \rangle_\alpha^+ + \langle \bar{\psi} e^{i\beta\gamma_5} \psi \rangle_\alpha^-],$$

$$\langle \bar{\psi} e^{i\beta\gamma_5} \psi \rangle_\alpha^\pm = \lim_{m \rightarrow 0} v^{-1} Z_\alpha^\pm(m, \beta),$$

$$Z_\alpha^\pm(m, \beta) = \mathcal{N} \int_{\mathcal{F}_\alpha} D\psi D\bar{\psi} \exp\left\{-S + m \int_v dx \bar{\psi} e^{i\beta\gamma_5} \psi\right\},$$

where $(-)+$ corresponds to an (anti-)self-dual domain. A chiral transformation:

$$\psi = e^{-i(\beta/2)\gamma_5} \psi' \quad (\text{A1})$$

for a field ψ belonging to \mathcal{F}_α , namely, satisfying

$$i\rlap{-}/\partial(x) e^{i\alpha\gamma_5} \psi(x) = \psi(x),$$

leads to the transformed field ψ' satisfying

$$i\rlap{-}/\partial(x) e^{i(\alpha-\beta)\gamma_5} \psi'(x) = \psi'(x),$$

so that ψ' belongs to $\mathcal{F}_{\alpha-\beta}$. Performed in the integral, this chiral transformation results in

$$Z_\alpha^\pm(m, \beta) = e^{i\Gamma(\beta)} Z_{\alpha-\beta}^\pm(m, 0) \quad (\text{A2})$$

where the phase Γ is fixed by β independence of $Z_\alpha^\pm(0, \beta)$ and the result for the fermionic determinant

$$Z_\alpha^\pm(0, 0) = \exp(\pm iq \arctan[\tan(\alpha)]),$$

which gives

$$\Gamma(\beta) = \pm 2 \arctan[\tan(\beta)]. \quad (\text{A3})$$

Thus, collecting all together, we get

$$Z_\alpha^\pm(m, \beta) = \exp\{\pm iq \arctan[\tan(\alpha)]\} \\ + v m \exp(\pm i(\alpha - \beta)) \mathfrak{N}.$$

In the presence of the θ term this gives

$$\langle \bar{\psi} e^{i\beta\gamma_5} \psi \rangle_\alpha^\pm = -e^{\pm iq(\arctan[\tan(\alpha)] - \theta)} [\cos(\alpha - \beta) \\ \pm i \sin(\alpha - \beta)] \mathfrak{N},$$

which finally, after summing self-dual and anti-self-dual configuration, leads to

$$\langle \bar{\psi} e^{i\beta\gamma_5} \psi \rangle_\alpha = -e^{\ln \cos\{q(\arctan[\tan(\alpha)] - \theta)\}} \mathfrak{N} \cos(\alpha - \beta).$$

Finally using this result for the complete calculation with $N \rightarrow \infty$ domains and integration over angles α_j associated with the j th domain, we get

$$\langle \bar{\psi} e^{i\beta\gamma_5} \psi \rangle = -\mathfrak{N} \sum_{kl} \cos(\alpha_{kl}(\theta) - \beta),$$

where the sum spans all 2π -inequivalent minima $\alpha_{kl}(\theta)$ of the free energy density, explicitly given in Eq. (18).

In particular, the pseudoscalar condensate corresponds to $\beta = \pi/2$ and thus reads

$$\langle \bar{\psi} i\gamma_5 \psi \rangle = N_f \mathfrak{N} \sum_{kl} \sin(\alpha_{kl}(\theta)).$$

It should be stressed here again, that for any θ and β

$$\sum_{kl} \cos(\alpha_{kl}(\theta) - \beta) \equiv 0.$$

We see that the θ dependence of the scalar condensate ($\beta = 0$) for different minima of the free energy density is given by $\cos(\alpha_{kl}(\theta))$ while the dependence of the pseudo-scalar condensate ($\beta = \pi/2$) is described by $\sin(\alpha_{kl}(\theta))$, as shown in Figs. 3 and 4.

The crucial point in this derivation is that the chiral transformation Eq. (A1) changes the space of integration and simultaneously generates a phase Γ in Eq. (A2). This phase is fixed in the form of Eq. (A3) by substituting $m = 0$ into Eq. (A2)

$$Z_\alpha^\pm(0, \beta) = e^{i\Gamma(\beta)} Z_{\alpha-\beta}^\pm(0, 0),$$

and taking into account the known explicit form of $Z_{\alpha-\beta}^\pm(0, 0)$ and $Z_\alpha^\pm(0, \beta)$, where the latter does not depend on β by construction.

APPENDIX B: OTHER DERIVATIONS OF THE DASHEN PHENOMENON

1. Anomalous Ward identities

We summarize the salient aspects of [5] and related works. Denote by $J_{\mu 5}$ the singlet axial vector current renormalized gauge invariantly. Its divergence gives the anomaly. Inserting this current into Green's functions with a composite operator consisting of a product of local observables $O_k(x_k)$, taking the divergence and using the anomaly one obtains

$$\begin{aligned} \partial_x^\mu T \langle 0 | J_{\mu 5}(x) \prod_k O_k(x_k) | 0 \rangle &= 2N \partial_x^\mu T \langle 0 | K_\mu(x) \prod_k O_k(x_k) | 0 \rangle \\ &\quad - \sum_l \chi_l \delta^{(4)}(x - x_l) T \\ &\quad \times \langle 0 | \prod_k O_k(x_k) | 0 \rangle. \end{aligned} \quad (\text{B1})$$

The quantity K_μ in the first term of the right-hand side is the well-known Chern-Simons current arising from the anomaly. The second term arises from commuting the divergence through the T product, which generally gives a commutator of the operators O_k with the axial charge, and then rewriting that commutator in terms of chiralities χ_k corresponding to O_k which are defined via the eigenvalue-like relation

$$[Q_5, O_k] = -\chi_k O_k. \quad (\text{B2})$$

The charge Q_5 does not correspond to $J_{\mu 5}$ but rather to the gauge-dependent, conserved axial current. Despite the gauge dependence of Q_5 , chiralities of Eq. (B2) are renormalization group and gauge invariant [5]. For a right-handed quark field $\chi = 1$. The condition for avoiding a $U(1)$ boson is that the left-hand side of Eq. (B1) vanishes at zero momentum transfer. Taken between θ vacua, one can rewrite the Chern-Simons current contribution (due to its connection to topological charge density) on the right-hand side via a derivative with respect to θ yielding

$$0 = \left[2N_f i \frac{\partial}{\partial \theta} - \sum_l \chi_l \right] T \langle 0 | \prod_k O_k(x_k) | 0 \rangle. \quad (\text{B3})$$

Now one chooses the local operator product $\bar{q}q$ such that the sum of chiralities is $\sum_l \chi_l = 2$. One extracts then the relation

$$\left(iN_f \frac{\partial}{\partial \theta} - 1 \right) \langle 0 | \bar{u}_L u_R | 0 \rangle = 0 \quad (\text{B4})$$

for example. This can be trivially solved for the condensate. The next step is to recognize the condensate here as an element of the matrix of condensates which break the nonsinglet chiral symmetry

$$\langle 0 | (\bar{q}_L)_i (q_R)_j | 0 \rangle = C V_{ij}.$$

This matrix can be brought by chiral rotations into a form $\text{diag}(e^{i\phi_i})$. The real angles ϕ_i parametrizing the matrix

now carry the θ dependence of the condensate. Inserting this into Eq. (B4) gives

$$\sum_{i=1}^{N_f} \left(N_f \frac{\partial \phi_i}{\partial \theta} - 1 \right) = 0$$

whose solution is

$$\sum_{i=1}^{N_f} \phi_i - \theta = 0. \quad (\text{B5})$$

This equation should be understood here as a direct consequence of the requirement that no zero mass boson couple to the gauge-invariant axial vector current.

The above considerations should be repeated in the presence of such a perturbation matrix of masses m_i for each flavor

$$\langle \epsilon H' \rangle = \sum_{i,j=1}^{N_f} m_i (V_{ij} + V_{ij}^\dagger) = 2 \sum_{i=1}^{N_f} m_i \cos \phi_i. \quad (\text{B6})$$

According to Dashen's theorem, the true vacuum is found by minimizing a quark mass term with respect to small chiral rotations about this configuration, meaning shifting ϕ_i under the cosine by infinitesimal ω_i . Minima are determined by the conditions

$$m_i \sin \phi_i = \text{independent of } i \equiv \lambda, \quad \cos \phi_i > 0. \quad (\text{B7})$$

To give an explicit solution assume $N_f = 2$ with degenerate quark masses. Then the consequence of Dashen's theorem Eq. (B7) gives $\sin \phi_i = \lambda/m$. Solutions consistent with Eq. (B7) are $\phi_i = \phi \in [-\pi/2, \pi/2]$ modulo 2π , with $\phi = \arcsin \lambda/m$. The absence of a Goldstone boson Eq. (B5) gives $\phi_1 + \phi_2 = \theta$. Combining these gives the result that the symmetry breaking term and thus the condensate is $|\cos(\theta/2)|$. Essentially the absolute value appears because the cosine may not change sign, due to Eq. (B7), as θ varies. Out of this emerges that the periodicity of θ is 2π . For general N_f with degenerate quark masses the corresponding result is that the condensate is proportional to $\cos[\theta(\text{mod } 2\pi)/N_f]$.

2. Large N_c approach

Now we briefly summarize how identical results are obtained in the large N_c approach of Witten and Veneziano-Di Vecchia [6]. An $N_f \times N_f$ unitary field U , parametrized as $U = U_0 \exp(i\pi^a t^a)$ with N_f^2 meson (nonsinglet and singlet) fields π^a , is considered: the $U(N_f)$ generators t^a include the identity matrix as well as the usual $SU(N_f)$ generators. An effective Lagrangian for U with chiral and axial $U(1)$ symmetry broken is

$$\mathcal{L} = \frac{F_\pi^2}{2} \left(\text{Tr} \partial_\mu U \partial_\mu U^\dagger + \text{Tr} (\mathcal{M} U + \mathcal{M}^\dagger U^\dagger) - \frac{a}{N_c} \times (-i \ln \det U)^2 \right)$$

where the first term is a kinetic term, the second a mass, and the third term is designed to only yield a term quadratic in the singlet field and is consistent with large N_c counting rules. The mass matrix \mathcal{M} is then diagonalized by an $SU(N_f) \times SU(N_f)$ transformation (corresponding to the action on the quark mass matrix) to the form

$$\mathcal{M} = e^{i\theta/N_f} M$$

with $M = \text{diag}(\mu_i^2)$. The μ_i^2 are combinations of the squares of the meson masses but are linear in the corresponding quark masses m_i , $\mu_i^2 \propto m_i$, generalizing the Gell-Mann–Oakes–Renner relationship and containing the quark condensates—see [22] for explicit formulas. The diagonalization leads to a corresponding phase transformation on the U field: $U \rightarrow e^{-i\theta/N_f} U$ such that the $\ln \det$ term undergoes a shift θ . The aim is now to minimize the effective potential to find the vacuum configurations. This is aided by considering a diagonal U parametrized as $\text{diag}(e^{i\phi_i})$ where the ϕ_i are complicated functions of the meson fields π^a . This leads to the potential

$$V(\phi_i) = F_\pi^2 \left[-\sum_i \mu_i^2 \cos \phi_i + \frac{a}{2N_c} \left(\sum_i \phi_i - \theta \right)^2 \right].$$

The terms with μ_i^2 evidently arise from the separate phases in U and thus after expanding the ϕ_i in powers of the meson fields π^a will give mass terms for the $N_f^2 - 1$ non-singlet mesons. The last term incorporates only information about the overall phase of U ; the corresponding expansion to second order in π^a will reflect the mass of

the singlet $U(1)$ state. That this is taken to be large compared to the other $N_f^2 - 1$ is now input at this point. One now minimizes with respect to the angles ϕ_i (Dashen's theorem) giving

$$\mu_i^2 \sin \phi_i = \frac{a}{N_c} \left(\sum_{j=1}^{N_f} \phi_j - \theta \right).$$

Evidently then one has again

$$\mu_i^2 \sin \phi_i = \text{independent of } i$$

identical to Eq. (B7). On the other hand, taking the first $N_f^2 - 1$ mesons to be light, the only way to minimize the potential for a heavy $U(1)$ boson is to constrain the term with factor a/N_c to be exactly zero, namely

$$\sum_i \phi_i - \theta = 0$$

which is identical to the condition from anomalous Ward identities—no surprise since the effective Lagrangian is engineered to satisfy these identities. Implementing these conditions leads to the identical dependence on θ discussed in the previous section, which now appears in the potential at its minima

$$V(\phi_i)_{\min} = -F_\pi^2 \sum_i \mu_i^2 \cos \phi_i |_{\min}.$$

Since the quark condensates reside in the μ_i^2 an identical dependence on θ as that found using anomalous Ward identities emerges. The dependence involves $\cos(\theta/N_f)$ now because of the way the U field transforms under chiral transformations in terms of the θ parameter: $\ln \det U \rightarrow \ln \det U - i\theta$ and there is no relative factor of 2 between the sum of the phases of U and θ .

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