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

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Abstract

A non-zero CP-violating θ parameter is treated in the domain model which assumes a cluster-like vacuum structure whose units are characterised 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 θ = π 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.

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

\[ S_\theta = i q \theta, \quad q = \frac{g^2}{32\pi^2} \int d^4 x F_{\mu\nu} \tilde{F}^{\mu\nu}. \]  

A remarkable feature of such a term in the presence of spontaneously broken chiral symmetry is the Dashen phenomenon \[\Pi\]: this explicit breaking of CP can become spontaneous due to vacuum doubling at the point θ = π. This value falls outside the physically relevant range 0 ≤ θ ≤ 10^{-9} to which θ is constrained by the neutron dipole moment \[\mathbf{2}\] and current algebra \[\mathbf{3}\]. Nonetheless, the Dashen phenomenon is a constraint on self-consistent models of the non-perturbative QCD vacuum. The statement of the problem related to the Dashen phenomenon as well as the question about periodic dependence of observables in θ acquire full sense only if the values of q are not restricted to integers. In this paper we use the domain model \[\mathbf{4}\] 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 \[\mathbf{5}\] and effective chiral Lagrangians \[\mathbf{6}\] in the limit of large number of colours \[N_c\], which we shall describe below in more detail. Subsequent discussions of the Dashen phenomenon include \[\mathbf{5, 6, 7, 8, 9, 10, 11}\]. This phenomenon for θ ≠ 0 is intimately related to both the mechanism of spontaneous chiral symmetry breaking and the non-appearance of an axial U(1) pseudoscalar Goldstone boson as shown by the original works revealing it in QCD. In \[\mathbf{5}\] the key tool is the generalisation 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 flavour SU(2)_L × SU(2)_R Ward identity (which gives the Gell-Mann–Oakes–Renner relation) leads to a non-zero chiral condensate as the output. In the axial U(1) channel (where the anomaly figures) and θ = 0 the phenomenological input is now the absence of a light meson, with the output that topological charge q must be fractional. With θ ≠ 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 θ = π. In the large N_c approach the same data is turned around. An effective Lagrangian for mesons is written down for N_c → ∞ which assumes chiral symmetry breaking and the anomaly. The output for θ = 0 includes the famous relation between the topological susceptibility and various meson masses. For θ ≠ 0 again the Dashen phenomenon emerges.

However these approaches do not unveil the actual mechanism of non-perturbative vacuum properties such as confinement and spontaneous chiral symmetry breaking. The domain model \[\mathbf{4}\] 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 domain-like gluon fields, and out of
this both vacuum and mesonic properties are derived. In previous works both confinement \( \mathbb{1} \) and chiral symmetry realisation \( \mathbb{12} \) \( \mathbb{13} \) have been studied for this vacuum ansatz. The 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 flavour \( SU(N_f)_L \times SU(N_f)_R \) chiral symmetry in turn are spontaneously broken with a quark condensate arising due to the asymmetry of the spectrum of Dirac operator in the domain background. An estimate of pseudoscalar and vector meson masses of observables such as the condensate arises as output appearing for which the vacuum doubling occur. As with \( \mathbb{6} \) and \( \mathbb{12} \), 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 realisation of chiral symmetry for \( \theta \neq 0 \). In the appendices we review and compare our results with the approaches of \( \mathbb{12} \) and \( \mathbb{13} \).

II. REVIEW OF CHIRAL SYMMETRY IN THE DOMAIN MODEL

For motivation and a detailed description of the domain model we refer the reader to \( \mathbb{13} \). The essential definition of the model is given in terms of the following partition function for \( N \to \infty \) domains of radius \( R \)

\[
Z = \mathcal{N}_\Sigma \lim_{V,N \to \infty} \int \frac{d^4z_i}{V} \int_0^{2\pi} d\varphi_i \int_0^\pi d\theta_i \sin \theta_i \int d\Sigma_i \ldots = \frac{1}{48\pi} \int_0^\infty d\xi_i \sum_{l=0}^{2.4.5} \delta(\xi_i - (2l + 1)\pi/6) \times \int_0^\pi d\omega_i \sum_{k=0}^{\text{max}} \delta(\omega_i - \pi k) \ldots ,
\]

where \( (\theta_i, \varphi_i) \) are the spherical angles of the chromomagnetic field, \( \omega_i \) is the angle between chromoelectric and chromomagnetic fields and \( \xi_i \) is an angle parametrising the colour orientation.
This partition function describes a statistical system of domain-like structures of density $v^{-1}$, where the volume of a domain is $v = \pi^2 R^4/2$. Each domain is characterised 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, colour 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 $\Lambda_{QCD}$ and, eventually, to the fundamental scale $\Lambda$ (19, 20). 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 $\sigma = B f(\pi BR^2)$ where $f$ is given for colour $SU(2)$ and $SU(3)$ in $\Lambda$. 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 $\Lambda$ these parameters are fixed to be $\sqrt{B} = 947$ MeV, $R = (760$ MeV)$^{-1} = 0.26$ fm with the average absolute value of topological charge per domain turning out to be $q = 0.15$ and the density of domains $v^{-1} = 42$ fm$^{-4}$. The topological susceptibility then turns out to be $\chi = (197$ MeV)$^4$, comparable to the Witten-Veneziano value $\Phi$. The eigenvalue problem

$$D\psi(x) = \lambda\psi(x),$$

with boundary condition Eq. (3) was studied in $\Lambda$. With the domain background field the solution to this problem reveals an asymmetric spectrum, exhibiting the broken chiral symmetry through the bag-like boundary condition, and thus none of the eigenmodes is chiral. However at the centre 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 $\Lambda$ we computed the distribution of values of the local chirality parameter of $\eta$ in a chirally symmetric ensemble revealing qualitatively similar behaviour to the double-peak structure seen on the lattice $\Lambda$, which is taken to be indicative of spontaneously broken chiral symmetry.

The $\alpha$-dependent part of the free energy density was computed in $\Lambda$ using zeta function regularisation, with an imaginary part arising

$$\Im F = \pm \frac{\eta}{v} \arctan(\tan(\alpha))$$

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 $\pi n$ periodic in $\alpha$. This is the Abelian anomaly as observed within the context of bag-like boundary conditions by $\Lambda$ and is consistent with $\Lambda$ albeit not generated from purely chiral zero modes but the chiral properties of non-zero modes.

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

$$e^{-\nu NF} = N \int_{-\infty}^{\infty} \cos v \Im F(\alpha)) + O(1/N).$$

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

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

In the thermodynamic limit $N \to \infty$ the solutions to the above equation for $\alpha_{\text{min}}$ 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 minimise 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 $\alpha$-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 $\Lambda$)

$$F = \frac{i}{v} \arctan(\tan(\alpha)) - m\pi e^{i\alpha} + O(m^2),$$

$$\eta = \frac{1}{\pi^2 R^3} \sum_{k=1, z=1, z=2}^{\infty} \frac{k}{k+1} |M(1, k+2, z) - z M(1, k+3, -z) - 1|,$$

where the quantity $\eta > 0$ 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 $\Lambda$. 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 $\alpha_{\text{min}}$ are not modified by the leading order term, linear in $m$. The quark condensate is extracted from the free energy in the standard way

$$\langle \bar{\psi}(x)\psi(x) \rangle = -\lim_{N \to 0} N \to \infty \lim_{m \to 0} \frac{1}{vN} \frac{d}{dm} e^{-vN\mathcal{F}(m)}$$

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 flavours the fermion boundary condition in Eq. (3), explicitly breaks all chiral symmetries, flavour singlet and non-singlet (see also [14]). Thus integrating over all $\alpha$ 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 generalised to include flavour non-singlet angles, $\alpha \to \alpha + \beta^i T^a/2$, with $T^a$ the $N_f^2 - 1$ generators of the pure gluonic characteristics of 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 Non-Zero $\theta$

Now we include the CP-violating parameter in the model by the additional term Eq. (11) in the action, which contributes a pure phase to the weight factor in Euclidean space. Integrating over $N_f$ fermions with infinitesimally small masses $m_1 = \cdots = m_N \equiv m$ in a domain ensemble gives for the free energy density per domain

$$F = -v^{-1} \ln \cos q[W_{N_f} - \theta] - m^3 \sum_{i=1}^{N_f} \cos \Phi_i,$$

where

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

$$\Phi_i = \alpha + B_i$$

$$B_1 = 0 \text{ for } N_f = 1,$$

$$B_1 = \frac{|\beta|}{2}, \ B_2 = -\frac{|\beta|}{2}, \text{ for } N_f = 2,$$

and

$$B_3 = b^3 + b^3/\sqrt{3}, \ B_2 = -b^3 + b^3/\sqrt{3},$$

$$B_3 = -2b^3/\sqrt{3}, \text{ for } N_f = 3.$$
Here $\alpha$ is the $U(1)$ chiral angle, $\beta$ are the non-singlet chiral angles for $N_f=2$, and $b_3$ and $b_8$ are certain functions of the eight non-singlet chiral angles $\beta^a$ 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 $SU(2)$ flavour sectors. For $N_f > 2$ the analogous functions are $B_1, \ldots, B_{N_f}$. For any number of flavours $N_f$ the functions $B_i$ have the property that

$$\sum_{i=1}^{N_f} B_i = 0$$

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

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

The “arctan tan” structure in Eq. (10) manifests the periodicity of the free energy for arbitrary topological charge $q$. We could write

$$W_{N_f} = \sum_{i=1}^{N_f} \text{arctan}[\tan \Phi_i] = N_f \alpha \text{ (mod } \pi)$$  \hspace{1cm} (16)

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

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

$$\alpha_{kl}(\theta) = \frac{\theta}{N_f} + \frac{2\pi l}{qN_f} + \frac{\pi k}{N_f} \quad (k \in \mathbb{Z}, l \in \mathbb{Z}), \hspace{1cm} (18)$$

to the equation

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

Evidently there are multiple solutions arising from the various periodic functions appearing in Eq. (19). 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 flavour non-singlet chiral angles, as discussed above, and thus the free energy displays continuous degeneracy with respect to these angles.

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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 $2\pi$-periodic copies of one of the already identified vacua. For instance, for $N_f=1$ and $q = .15$ 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 $2\pi$-periodic with respect to $\theta$:

$$\alpha_{kl}(\theta + 2\pi m) \rightarrow \alpha_{k,l}(\theta), \quad k' = k + 2m, \hspace{1cm} (20)$$

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

FIG. 4: The pseudo-scalar quark condensate as a function of $\theta$ for $N_f = 3$ and $q = .15$ in units of $\hbar$. The meaning of dashed and solid lines is the same as in Fig. 2.

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

$$qW_{N_f} = N_f q\alpha + O(\alpha^2) \quad \text{for } \alpha \rightarrow 0,$$ \hspace{1cm} (17)

which coincides with the standard form of axial anomaly in the Fujikawa derivation (Note that $\alpha$ here is twice the angle of chiral transformation used in the Fujikawa’s calculation of anomaly [12]).

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Evidently there are multiple solutions arising from the various periodic functions appearing in Eq. (19). 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 flavour non-singlet chiral angles, as discussed above, and thus the free energy displays continuous degeneracy with respect to these angles.

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FIG. 3: The pseudo-scalar quark condensate as a function of $\theta$ for $N_f = 1$ and $q = .15$ in units of $\hbar$. The meaning of dashed and solid lines is the same as in Fig. 2.
Switching on the infinitesimal mass term in Eq. (3) lifts the degeneracy due to different values of the symmetry breaking term

$$V_m = -m \Phi \sum_{i} \cos(\Phi_i(\theta))$$  \hspace{1cm} (21)

in the free energy for different $\Phi_i = \alpha + B_i(\beta^a)$. This introduces non-singlet angle dependence into the free energy, which must now also be minimised with respect to the $\beta^a$. To this end we expand $V_m$ in small fluctuations in the $B_i$ and look for minima, bearing in mind the constraint Eq. (13). The condition that $V_m$ have stationary points leads to the condition

$$\sin \Phi_i \text{ independent of } i$$  \hspace{1cm} (22)

while the condition that this leads to a minimum forces

$$\cos \Phi_i > 0.$$  \hspace{1cm} (23)

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

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

Thus to guarantee a minimum with respect to non-singlet 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. (10), 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 flavour 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 $\theta$ dependence of the quark condensate is given by

$$\langle \bar{\psi}(x)\gamma_5\psi(x)\rangle_{\alpha_{kl}(\theta)} = -N_f R \cos(\alpha_{kl}(\theta))$$

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 $\theta$ for the minima which are not 2$\pi$-equivalent. Critical values of $\theta$ 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 behaviour of pseudoscalar condensate as a function of $\theta$

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

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

The plots for one and three flavours respectively are given in Figs. 3 and 4 again with $q = 0.15$. The pseudoscalar condensate is discontinuous at the critical values of $\theta$ 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 $\theta$ where two different minima are degenerate, thus displaying a two-fold degeneracy of the vacuum in the presence of a mass.

There are two conditions for critical $\theta$. The first one is obviously

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

where $k$ and $l$ should not be equal to zero simultaneously and without loss of generality we have taken $\alpha_{00}$ on the RHS. Thus

$$\theta_{\text{crit}} = \pi k + \frac{l\pi}{q} \text{ (mod 2$\pi$)}.$$  \hspace{1cm} (mod 2$\pi$)

For a given $q$ this defines set of values of $\theta_{\text{crit}}$ where several vacua are degenerate. This set is independent of number of flavours $N_f$. Furthermore, we are interested only in those $\theta_{\text{crit}}$ which minimise the term linear in mass, which is the second condition for $\theta_{\text{crit}}$. 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 2$\pi$-periodicity of amplitudes in $\theta$ and vacuum doubling with spontaneous CP violation at certain critical values of $\theta$, in particular $\theta = \pi$, are obtained for any number of light flavours $N_f$ 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 iso-vector and iso-singlet 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, characterised by a finite correlation length. In this paper and in previous works it has been shown on a semi-quantitative level that such vacuum fields can reproduce all of the qualitatively important features of the QCD vacuum associated with confinement and chiral symmetry realisation.

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

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

from Eq. (19). Resolving the arctan tan structure brings us to the same form as in Eq. (24), when $\phi_i$ and $\Phi_i$ 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 non-singlet meson fields there are contained in $U(N_f)$ matrices but diagonalised 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 $U(N_f)$ flavour matrices $\exp[i(\alpha + \beta^a T^a)/2]\gamma_5$ which are similarly diagonalised 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].

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 summarised the salient features of these approaches in Appendix B.

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 non-singlet meson fields there are contained in $U(N_f)$ matrices but diagonalised 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 $U(N_f)$ flavour matrices $\exp[i(\alpha + \beta^a T^a)/2]\gamma_5$ which are similarly diagonalised by special unitary matrices.

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The significance of our result in comparison to [5] is that the domain model assumes the dominance of specific class of nonperturbative gluon configurations in the QCD vacuum, leading to a constraint on the sum of the aforementioned angles $\phi_i$ and the theta parameter:

$$\sum_{i=1}^{N_f} \phi_i = \theta$$

In both [5, 10], the input that there be no such boson leads to a constraint on the sum of the aforementioned angles $\phi_i$ and the theta parameter:

$$\sum_{i=1}^{N_f} \phi_i = \theta$$

from Eq. (19). Resolving the arctan tan structure brings us to the same form as in Eq. (24), when $\phi_i$ and $\Phi_i$ 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 non-singlet meson fields there are contained in $U(N_f)$ matrices but diagonalised 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 $U(N_f)$ flavour matrices $\exp[i(\alpha + \beta^a T^a)/2]\gamma_5$ which are similarly diagonalised by special unitary matrices.
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 particular, the absence of a pseudoscalar U(1) boson is input simultaneously to obtain the theta dependence, while the responsible vacuum structure is unknown.

The present work can be generalised for the case of non-degenerate quark masses in the presence of the theta term for which an analysis using anomalous Ward identities is given in [2]. Because of the above-noted similarities with the domain model the condensate dependence on \( \theta \) 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 minimised by \( \theta = 0 \), but there is no reason within the model to demand the minimisation of the free energy with respect to \( \theta \), 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 \( \theta \) in any finite interval. We shall analyse this intriguing possibility in a separate publication.

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APPENDIX A: PSEUDO-SCALAR CONDENSATE

We treat here \( N_f = 1 \) and the integral for one domain for simplicity; the generalisation is straightforward. Consider

\[
\langle \bar{\psi} e^{i\beta \gamma_5} \psi \rangle_{\alpha} = \frac{1}{2} \left( \langle \bar{\psi} e^{i\beta \gamma_5} \psi \rangle^+_{\alpha} + \langle \bar{\psi} e^{i\beta \gamma_5} \psi \rangle^-_{\alpha} \right)
\]

\[
\langle \bar{\psi} e^{i\beta \gamma_5} \psi \rangle^\pm_{\alpha} = \lim_{m \to 0} v^{-1} Z^\pm_{\alpha}(m, \beta)
\]

\[
Z^\pm_{\alpha}(m, \beta) = \mathcal{N} \int_{\mathcal{F}_\alpha} D\psi D\bar{\psi} \exp \left\{ -S + m \int_{\psi} \bar{\psi} e^{i\beta \gamma_5} \psi \right\},
\]

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

\[
\psi = e^{-i\frac{\eta}{2} \gamma_5} \psi'
\]

for a field \( \psi \) belonging to \( \mathcal{F}_{\alpha} \), namely satisfying

\[
i \gamma(x)e^{i\gamma_5} \psi'(x) = \psi'(x),
\]

leads to the transformed field \( \psi' \) satisfying

\[
i \gamma(x)e^{i\gamma_5} \psi'(x) = \psi'(x),
\]

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

\[
Z^\pm_{\alpha}(m, \beta) = e^{i\Gamma(\beta)} Z^\pm_{\alpha - \beta}(m, 0)
\]

where the phase \( \Gamma \) is fixed by \( \beta \)-independence of \( Z^\pm_{\alpha}(0, \beta) \) and the result for the fermionic determinant

\[
Z^\pm_{\alpha}(0, 0) = \exp(\pm iq \arctan[\tan(\alpha)])
\]

which gives

\[
\Gamma(\beta) = \pm 2 \arctan[\tan(\beta)].
\]

Thus, collecting all together, we get

\[
Z^\pm_{\alpha}(m, \beta) = \exp \left\{ \pm iq \arctan[\tan(\alpha)] \right\} + \text{const.}
\]

In the presence of the \( \theta \)-term this gives

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

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

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

Finally using this result for the complete calculation with \( N \to \infty \) domains and integration over angles \( \alpha \) associated with \( j \)-th domain, we get

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

where the sum spans all \( 2\pi \)-invariant minima \( \alpha_{kl}(\theta) \) of the free energy density, explicitly given in Eq. (A3).

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

\[
\langle \bar{\psi} i\gamma_5 \psi \rangle = N \sum_{kl} \sin(\alpha_{kl}(\theta))
\]

It should be stressed here again, that for any \( \theta \) and \( \beta \)

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

We see that the \( \theta \)-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 pseudoscalar 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 \( \Gamma \) in Eq. (A2). This phase is fixed in the form of Eq. (A3) by substituting \( m = 0 \) into Eq. (A2)

\[
Z^\pm_{\alpha}(0, 0) = e^{i\Gamma(\beta)} Z^\pm_{\alpha - \beta}(0, 0),
\]

and taking into account the known explicit form of \( Z^\pm_{\alpha - \beta}(0, 0) \) and \( Z^\pm_{\alpha}(0, \beta) \), where the latter does not depend on \( \beta \) by construction.
APPENDIX B: OTHER DERIVATIONS OF THE DASHEN PHENOMENON

1. Anomalous Ward identities

We summarise the salient aspects of [5] and related works. Denote by $J_{\mu 5}$ the singlet axial vector current renormalised 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

$$
\partial^\mu T(0)J_{\mu 5}(x)\prod_k O_k(x_k)|0\rangle =
2N\partial^\mu T(0)K_\mu(x)\prod_k O_k(x_k)|0\rangle
- \sum_l \chi_l \delta^{(4)}(x - x_l)T(0)\prod_k O_k(x_k)|0\rangle
$$

(B1)

The quantity $K_\mu$ in the first term of the RHS 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 $\chi_k$ corresponding to $O_k$ which are defined via the eigenvalue-like relation

$$
[Q_5, O_k] = -\chi_k O_k.
$$

(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 renormalisation group- and gauge-invariant [6]. For a right handed quark field $\chi = 1$. The condition for avoiding a $U(1)$ boson is that the LHS of Eq. (B1) vanishes at zero momentum transfer. Taken between $\theta$ vacua, one can rewrite the Chern-Simons current contribution (due to its connection to topological charge density) on the RHS via a derivative with respect to $\theta$ yielding

$$
0 = [2Nf_i \frac{\partial}{\partial \theta} - \sum_l \chi_l] T(0)\prod_k O_k(x_k)|0\rangle.
$$

(B3)

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

$$
(iNf \frac{\partial}{\partial \theta} - 1)(0)|\bar{u}_L u_R|0\rangle = 0
$$

(B4)

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

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

This matrix can be brought by chiral rotations into a form $\text{diag}(e^{i\phi_i})$. The real angles $\phi_i$ parametrising the matrix now carry the $\theta$ dependence of the condensate. Inserting this into Eq. (B3) gives

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

whose solution is

$$
\sum_{i=1}^{N_f} \phi_i - \theta = 0.
$$

(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 flavour

$$
\langle tH' \rangle = \sum_{i,j=1}^{N_f} m_i (V_{ij} + V_{ji}^\dagger)
= 2 \sum_{i=1}^{N_f} m_i \cos \phi_i
$$

(B6)

According to Dashen’s theorem, the true vacuum is found by minimising a quark mass term with respect to small chiral rotations about this configuration, meaning shifting $\phi_i$ under the cosine by infinitesimal $\omega_i$. Minima are determined by the conditions

$$
m_i \sin \phi_i = \text{independent of } i \equiv \lambda
\cos \phi_i > 0.
$$

(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 $\phi_1 = \phi \in [-\pi/2, \pi/2]$ modulo $2\pi$, with $\phi = \arcsin \lambda/m$. The absence of a Goldstone boson Eq. (B6) 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 $\lambda$ varies. Out of this emerges that the periodicity of $\theta$ is $2\pi$. 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 summarise 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 $U$, parametrised as $U = U_0 \exp(i\pi a_t^a)$ with $N_f^2$ meson (non-singlet and singlet) fields $\pi^a$, 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

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

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 $M$ is then diagonalised 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 $\mu_i^2$ are combinations of the squares of the meson masses but are linear in the corresponding quark masses $m_i$, $\mu_i^2 \propto m_i$, generalising the Gell-Mann–Oakes–Renner relationship and containing the quark condensates - see [22] for explicit formulae. The diagonalisation 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 $\theta$. The aim is now to minimise the effective potential to find the vacuum configurations. This is aided by considering a diagonal $U$ parametrised as diag($e^{i\theta_i}$) where the $\phi_i$ are complicated functions of the meson fields $\pi^a$. 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 $\mu_i^2$ evidently arise from the separate phases in $U$ and thus after expanding the $\phi_i$ in powers of the meson fields $\pi^a$ 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 $\pi^a$ 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 minimises with respect to the angles $\phi_i$ ("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([23]). On the other hand, taking the first $N_f^2 - 1$ mesons to be light, the only way to minimise 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 $\theta$ discussed in the previous section, which now appears in the potential at its minima

$$V(\phi_i)_{\text{min}} = -F_\pi^2 \sum_i \mu_i^2 \cos \phi_i|_{\text{min}}.$$
[19] N.K. Nielsen, Nucl. Phys. B 120, 212 (1977).
[20] P. Minkowski, Nucl. Phys. B 177, 203 (1981).
[21] L. Bergamin, P. Minkowski, [hep-th/0003097] (2000); M. Leibundgut, P. Minkowski, Nucl. Phys. B 531, 95 (1998).
[22] A. Pich and E. de Rafael, Nucl. Phys. B 367, 313 (1991).