QCD at Large $\theta$ Angle and Axion Cosmology

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Abstract

We use the chiral Lagrangian to investigate the global properties of the $N$-flavor QCD vacuum as a function of the $\theta$ parameter. In the case of exact quark degeneracy we find evidence for first order phase transitions at $\theta = \pi \cdot$ (odd integer). The first order transitions are smoothed by quark mass splittings, although interesting effects remain at realistic quark masses. We emphasize the role of the $\eta'$ condensate in our analysis. Finally, we discuss the implications of our results on the internal hadronic structure of axion domain walls and axion cosmology.

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1 Introduction

The QCD Lagrangian may be augmented with the gauge invariant term $\theta \frac{G \tilde{G}}{32 \pi^2}$ which, despite being a total divergence, can have physical effects due to gauge field configurations with non-trivial topology. In nature this term appears to be absent (or at least small – $\theta \leq 10^{-10}$), but it is of theoretical interest to determine the effect such a term has on the theory. It is possible that understanding the effects of a non-zero $\theta$ angle may help determine why the term is absent in the strong interactions. In this paper we shall study the effects of adding a non-zero $\theta$ angle on the QCD vacuum assuming it does not change the pattern of chiral symmetry breaking $(SU(N)_L \otimes SU(N)_R \rightarrow SU(N)_V)$ in the quark sector. While it is possible that adding a non-zero theta term to QCD may have more dramatic effects, such as altering the nature of confinement [2,3], we consider ours to be the more conservative assumption. In fact, it can be shown [4] that some exactly solved softly broken supersymmetric gauge theories which confine by dyon condensation continue to do so for all $\theta \neq 0$. If the behaviour of QCD is smooth with changing $\theta$ then the low energy theory may be described in terms of the standard chiral Lagrangian formalism. Witten [5] has previously studied this possibility and shown that there may be first order phase transitions at $\theta = \pi$. He was particularly interested in the possibility of spontaneous CP violation at $\theta = \pi$ (note that although $\theta \neq 0$ in general violates CP, $\theta = \pi$ actually conserves CP). Creutz [6] further explored the phase structure of the mass degenerate chiral Lagrangian, demonstrating the existence of first order phase transitions at $\theta = n\pi$ ($n \in \text{odd integers}$). Here we develop these observations with further study of these phase transitions, concentrating in particular on the role of the $\eta'$ meson, and study their behavior in the presence of mass splitting in the quark sector. We find that even for realistic values of the quark masses interesting effects persist as $\theta$ is varied from 0 to $2\pi$. Finally, we discuss the implications of these phase transitions on axion models, in which $\theta$ is a dynamical variable. In particular, we investigate the internal hadronic structure of axion domain walls (previously studied by Huang and Sikivie [7]), and their coupling to thermal degrees of freedom in the early universe. We conclude that the domain walls can efficiently dissipate their kinetic energy and therefore contract away very rapidly after the QCD phase transition.

2 $N$ Degenerate Quark Flavors

As a first example we consider QCD with $N$ quark flavors and a non-zero $\theta$ angle

$$\mathcal{L} = -\frac{1}{4g^2}G^{\mu\nu}G_{\mu\nu} + \bar{\Psi}_i (i\gamma^\mu D_\mu - M)_{ij} \Psi_j + \theta \frac{32\pi^2}{1} \epsilon_{\mu
u\alpha\beta} G^{\mu\nu} G^{\alpha\beta}$$

However, in these models the low energy effective $\theta$ angle depends in a complicated fashion on the bare $\theta$ angle.
where $i$ runs over the $N$ flavors, and we shall take $M = m \mathcal{I}$. The bare Lagrangian has
an $SU(N)_L \otimes SU(N)_R \otimes U(1)_Y$ global flavor symmetry weakly broken by the small current
quark masses. The axial $U(1)$ symmetry of the classical theory is anomalous in the quantum
theory. Using the chiral Ward Identity associated with the $U(1)_A$ symmetry we may rotate
the $\theta$ term on to the quark mass matrix which becomes $M_{\theta} = M e^{i\theta/N}$.

We shall assume that for all $\theta$ the theory confines and breaks the chiral symmetry of the
quarks to the vector subgroup. At low energies the theory may then be described by the
standard $SU(N)_L \otimes SU(N)_R$ chiral Lagrangian

$$
\mathcal{L} = \frac{F^2}{4} \text{tr}(\partial^\mu U^\dagger \partial_\mu U) + \Sigma \text{Re} \text{tr}(M_{\theta} U^\dagger) ,
$$

where $U(x) = \exp(2i\pi a^T a / F)$ is an $SU(N)$ matrix. Taking a derivative with respect to $M_{ij}$
in (1) and (2) we note that

$$
\langle \bar{\Psi}_i \Psi_j \rangle = \Sigma \langle U_{ji}^\dagger \rangle ,
$$

so $U$ can be directly related to condensates of quark bilinears.

The behavior of the minimum of the potential with changing $\theta$ is easily determined when
$N = 2$ since the trace of a general $SU(2)$ matrix is real and the potential reduces to

$$
\epsilon_0 = -m \Sigma \cos(\theta/2) \text{Re} \text{tr}U \equiv -m \Sigma \cos(\theta/2) u ,
$$

where we have defined $u \equiv \text{Re} \text{tr}U$. The variable $u$ varies between $-1$ and $1$, and for
$\cos(\theta/2) \neq 0$ the potential energy is minimized at one of those values. These vacua corre-
spond to $U$ matrices

$$
U = \pm \begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix} .
$$

When $\theta = (\text{odd integer}) \cdot \pi$ the potential is exactly zero (at lowest order in the potential) and
all $U$’s are exactly degenerate. It is easy to see that at these values of $\theta$ there is a first order
phase transition with the vacuum jumping discontinuously between the two configurations (3). We show the form of the potential $V$ graphically in Figure 1 for varying $\theta$ and for the
set of configurations $U = \text{diag}(e^{i\alpha}, e^{-i\alpha})$ (non-zero $\alpha$ corresponds to a $\pi^0$ condensate). The
vertical axis in the figure is measured in units of $\Sigma m$. The first order phase transition at
$\theta = \pi$ is clear.

Creutz [6] has investigated the global behavior for general $N$. In this case there are $N$
distinct minima of the form

$$
U = e^{-2n\pi i/N} \mathcal{I} \quad n = 1, 2, \ldots N ,
$$

occurring for the special values of $\theta$

$$
\theta_n = 2n\pi \quad n = 1, 2, \ldots N .
$$
These minima are connected by N first order phase transitions at $\theta = (\text{odd integer}) \pi$. We note that the minima correspond to the vector flavor symmetry preserving diagonal SU(N) matrices. The $U(1)_A$ symmetry provides a simple understanding of the origin of the $N$ vacua in (3), which are characterized by bilinear quark condensates. The $U(1)_A$ symmetry of (3) is broken by the anomaly to a $Z_{2N}$ discrete symmetry acting on the quark fields. Therefore, discrete $Z_N$ transformations on the quark condensates relate equivalent vacua of the theory.

There is an important subtlety to discuss at this point. To include the effects of the $\theta$ angle in the chiral Lagrangian we have made a $U(1)_A$ rotation on the quark fields and moved the $\theta$ dependence into the quark mass matrix. To put the low energy Lagrangians of bare theories with different $\theta$ angles into the form of (2), different axial rotations have been made in each case. Before comparing the quark condensates in different models we must undo (or compensate for) this axial rotation. We denote the matrix of condensates in the original basis of (1) as $U_0 = e^{-i\phi/N} U$. In the original basis the overall phase of the quark condensate changes smoothly with $\theta$ and a discontinuous jump in the $\pi^0$ condensate occurs at $\theta = \pi$. This is shown in Figure 2 for the case of $N = 2$, where the $U_0$ is parametrized as

$$U_0 = e^{-i\phi/2} \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}.$$ (8)

After including the compensatory axial rotation, the vacua at $\theta = 0, 2\pi$ are now identical, and given by

$$U_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$ (9)
Similarly, in the $N$ flavor case the compensatory rotations also cancel the phase factors in (3). Thus in the original quark basis the $N$ vacua found by Creutz are actually the same vacuum and correspond to $U_0 = I$.

Figure 2: Phases of the vacuum $U_0$ matrix as a function of $\theta$ in the degenerate two flavor case.

In the two flavor case, for $\theta = \pi \pm \epsilon$, the (compensated) minima are respectively

$$U_0(\pi + \epsilon) = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix}, \quad U_0(\pi - \epsilon) = \begin{pmatrix} -i & 0 \\ 0 & -i \end{pmatrix} \quad (10)$$

Since they have an associated phase they violate CP. This model realizes the possibility discussed by Witten that at $\theta = \pi$ there may be spontaneous CP violation by the occurrence of two CP violating vacua. (CP is not explicitly violated when $\theta = \pi$ since physics is invariant to $2\pi$ shifts in $\theta$, and CP acts by changing the sign of any phase in the theory, $\theta = \pm \pi$ are equivalent.)

3 Large $N_c$

To better understand the physical implications of the vacuum dependence on $\theta$ it is helpful to consider the problem in an $SU(N_c)$ gauge theory at large $N_c$. In this context the phase of $U$ can be identified with a condensate in the $\eta'$ field. It is well known that the anomaly in the $U(1)_A$ symmetry is the result of the quark triangle graph which is suppressed at leading order in $1/N_c$. Thus at large $N_c$ the full $U(N)_L \otimes U(N)_R$ global symmetry on the
fermions is restored. The fermion condensates break the symmetry to $U(N)V$ and there are $N^2$ goldstone bosons with the new state being identified with the $\eta'$. At $O(1/N_c)$ in the $N_c$ expansion the $\eta'$ acquires a small mass. If for a given large value of $N_c$ we take the quark masses to zero then this subleading term can dominate the $\eta'$ mass. In [8] it was argued that this is the limit most appropriate to realistic QCD. We can hope therefore to obtain some insight into the transition described above by looking to the large $N_c$ limit.

The effective theory at large $N_c$ is

$$L = \frac{F^2}{4} tr(\partial_\mu U^\dagger \partial^\mu U) + \Sigma Retr(MU^\dagger) - \frac{\tau}{2}(\phi - \theta)^2. \tag{11}$$

Here $U$ contains the $N^2$ goldstone degrees of freedom, and is no longer restricted to unit determinant. The additional phase degree of freedom corresponds to the $\eta'$ meson, with

$$detU(x) = e^{-i\phi(x)}$$

and

$$\phi(x) = -\frac{\sqrt{2N}}{F}\eta'.$$ \tag{12}

To obtain (11) we have performed an axial rotation on the bare Lagrangian to move the $\theta$ dependence into the mass matrix, then undone the rotation by absorbing $\theta$ with a shift in the $\eta'$ field. This redefinition of the phase of $U$ corresponds exactly to the previously discussed subtlety of ensuring that we compare theories with different $\theta$ in the same quark basis. It is important to note that the final term in (11) is only the first term in an expansion in $\phi - \theta$ of a function that is $2\pi$ periodic.

Restricting our attention again to the case $N = 2$ the potential of the large $N_c$ theory is

$$V = -\Sigma Retr(MU^\dagger) + \frac{\tau}{2}(\phi - \theta)^2. \tag{13}$$

We are interested in the case $\tau/\Sigma m \to \infty$, where the $\eta'$ is very heavy, and we expect to recover the analysis of the $SU(2)$ chiral Lagrangian above. The second term in the potential dominates and is minimized by $\phi = \theta$. As $\theta$ changes between 0 and $2\pi$ the phase of the mass matrix, which is the $\eta'$ condensate, behaves as in Figure 2. An ambiguity in the description arises here because a $\pi^0$ condensate corresponding to $\alpha = \pi$ has the same effect as an $\eta'$ condensate of $\phi = 2\pi$ on the matrix $U$ in (8). This ambiguity is resolved in the presence of mass splittings, as the discontinuities are smoothed, and one can resolve the different behaviors of the $\pi^0$ and $\eta'$ condensates. We discuss the effect of mass splittings below.
4 Mass Splitting

Returning to the $SU(N)$ chiral Lagrangian we may now consider the effects of splitting the quark masses. The potential is then

$$V = - \Sigma_i m_i \cos(\alpha_i - \theta/N) - \Sigma m_N \cos(\theta/N + \Sigma_i \alpha_i)$$  \hspace{1cm} (14)

As before we have made an equal axial rotation on each quark flavor to shift the $\theta$ angle onto the quark mass matrix. The minima are of the form

$$\langle U \rangle = \text{diag} \left( e^{i\alpha_1}, e^{i\alpha_2}, \ldots, e^{i\alpha_{N-1}}, e^{-i\sum_{i=1}^{N-1} \alpha_i} \right)$$ \hspace{1cm} (15)

If we take $m_N/m_i \to \infty$ the last term in (14) dominates and the heavy quark condensate acquires a phase $\sum_{i=1}^{N-1} \alpha_i = \theta/N$. In other words the phase of the $N$th diagonal element of $UM_\theta$ goes to zero corresponding to decoupling of the heavy quark and the problem reduces to that in which the $\theta$ angle has been rotated onto just the $N-1$ light quarks. This is why the strong CP problem cannot be solved by simply rotating the $\theta$ angle solely onto a heavy quark such as the top. In nature the charm, bottom and top quarks are sufficiently heavy that they essentially decouple from the $\theta$ dependence of the vacuum.

For intermediate mass splittings we must minimize (14). For $N = 2$ this is most easily done numerically. Minimizing (14) and rotating the resulting $U$ back to the quark basis of (1) we have

$$U_0 = e^{-i\theta/2} \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}.$$ \hspace{1cm} (16)

We show the phase $\alpha$ that minimizes the potential at varying $\theta$ for increasing mass splitting in Figure 3. The first order phase transition is smoothed out by the mass splitting and as $m_d/m_u \to \infty$ we recover the one flavor case for which there is a single vacuum.

![Figure 3: The phase $\alpha$ vs $\theta$ in the presence of mass splitting.](image-url)
With mass splittings there is only a single CP conserving minimum at $\theta = \pi$:

$$U_0 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$  

(17)

This minimum violates the vector symmetry of the model, however, this is just a reflection of the explicit breaking of that symmetry in the non-degeneracy of the quark masses. Furthermore, in this case one can easily see by examining the form of $U$ that both the $\eta'$ and the $\pi^0$ condensates are changing with $\theta$.

The three flavor case is more complicated. The minimization equations reduce to (with $U = \text{diag}(e^{i\alpha}, e^{i\beta}, e^{-i(\alpha + \beta)})$)

$$m_u \sin(\alpha - \theta/3) = m_d \sin(\beta - \theta/3) = -m_s \sin(\alpha + \beta + \theta/3)$$  

(18)

The behavior is most easily studied by displaying the solutions at $\theta = \pi$, where phase transitions are likely to occur. There are several types of solutions to (18). Trivial solutions occur when the sine functions are all simultaneously zero. For realistic quark masses ($m_u \sim 5 \text{ MeV}, m_d \sim 10 \text{ MeV}, m_s \sim 150 \text{ MeV}$) one of these solutions is the global (and only) minimum corresponding to the heavy strange quark having decoupled and the minimum closely resembles the $N = 2$ case with $m_u \neq m_d$ (See Figure 3). Non-trivial solutions were studied previously by Witten [5], and occur when the quark masses satisfy

$$m_u m_d \geq m_s |m_d - m_u|,$$  

(19)

which includes the degenerate mass limit discussed above. They satisfy

$$1 - \cos(\alpha + \beta + \pi/3) = \frac{m_u^2 m_d^2 - m_s^2 (m_d - m_u)^2}{2m_s^2 m_u m_d}.$$  

(20)

These latter solutions exhibit spontaneous CP violation. In this case the trivial solutions discussed above become points of inflection. Witten’s solutions are probably excluded for realistic values of the light quark masses.

As an explicit example we have examined the behavior with varying $\theta$ of the Large-$N_c$ effective Lagrangian. We used the physical $\eta, \eta'$ masses to determine $\tau/\Sigma = 200 \text{ MeV}$ and $m_s = 150 \text{ MeV}$. With such large values of $\tau$ and $m_s$ the $\tau$ and $m_s$ dependence of the solutions effectively decouples, and we are left with the behavior of the $SU(2)$ chiral Lagrangian. For example, taking $m_u = m_d = 7 \text{ MeV}$, we recover the first order transition of the degenerate two flavor case. Minimization in the $SU(3)$ degrees of freedom in $U = e^{-i\phi/3} \text{diag}(e^{i(\alpha + \beta)}, e^{i(-\alpha + \beta)}, e^{-i(2\beta)})$ leads to discontinuities in the $\pi^0, \eta$ and $\eta'$ condensates at $\theta = \pi$ (Figures 4,5).
Figure 4: The value of the potential at the minimum as a function of $\theta$ for the case of degenerate $u$ and $d$ quarks, $m = 7\,\text{MeV}$, $m_s = 150\,\text{MeV}$, $\tau/\Sigma = 200\,\text{MeV}$.

Figure 5: The condensates $\alpha \propto \pi^0$, $\beta \propto \eta$, $\phi \propto \eta'$ as functions of $\theta$.

If one moves away from $\theta = \pi$ one of the two solutions of the minimization equation (18) becomes the global minimum, whereas the other solution is a local minimum. By crossing $\theta = \pi$ the global minimum switches between the two branches. This description is valid in the vicinity of $\theta = \pi$. For $|\theta - \pi| > m_u/m_s$ the second (local) minimum disappears and there is only one (global) minimum. The situation is similar for a small mass splitting between $m_u$ and $m_d$, although Witten’s condition (19) is modified for $\theta \neq \pi$. Finally, for large mass splittings there is only one minimum of the potential for all values of $\theta$ (see also [6]).
5 Axion Cosmology

The results described above have some interesting implications for axion cosmology, particularly for non-trivial configurations like axion domain walls (ADWs). The internal structure of the ADW was investigated previously by Huang and Sikivie [7], who were the first to notice its internal $\pi^0$ structure. In this section we emphasize the additional $\eta, \eta'$ structure of the wall and the nature of the coupling of an ADW to thermal degrees of freedom below the QCD phase transition.

In axion models [1] the role of the $\theta$ parameter is played by a dynamical axion field $a$, whose potential energy is minimized at $\theta$ very close to zero, thus providing a solution to the strong CP problem. The models must exhibit an anomalous Peccei-Quinn symmetry, $U(1)_{PQ}$, at high energies, which is spontaneously broken at some scale $f_{PQ}$.

Because of the spontaneous breaking of a $U(1)$ symmetry, the cosmology of these models is somewhat involved. At temperatures below $f_{PQ}$, global cosmological strings are formed, which persist until the QCD chiral phase transition (unless inflation occurs with reheat temperature below $f_{PQ}$). At the QCD phase transition the degeneracy corresponding to different values of $\langle a \rangle/f_{PQ} \sim \theta$ is lifted, with the energy minimized at $\theta = 2\pi n$, $n \in \mathbb{Z}$ in the simplest (N=1) axion models. Since the axion field undergoes a ‘winding’ about the axis of the string, after the chiral phase transition the axion strings become connected by domain walls in which the axion field interpolates from $\theta = 0$ to $\theta = 2\pi$ over a lengthscale $m_a^{-1}$. Our earlier results imply that there are also domain walls in the $\pi^0, \eta$ and $\eta'$ condensates across the ADW. We note that the physical axion and Goldstone fields are obtained by diagonalizing the low energy mass matrix, see for example [9].

The subsequent evolution of a network of axion strings connected by domain walls was studied in [10], with the conclusion that the ADWs could persist for many horizon times and eventually even affect structure formation. This conclusion relies on the assumption that the ADW is extremely weakly coupled to the thermal background particles$.^4$ In [7] this assumption was justified by detailed calculations. However, only the $\pi^0$ component of the ADW was considered in [7], and in particular only the derivative couplings of the $\pi^0$ to nucleons. The derivative couplings lead to effects which are suppressed by the spatial derivative of the wall, which is $\sim m_a$ and hence very small.

There are additional interactions of the ADW with the thermal background which lead us to believe that, in fact, the ADW is strongly coupled and can rapidly dissipate excess energy. The relevant couplings are due to

- The internal $\eta, \eta'$ structure of the wall, which couples strongly to all hadronic thermal modes. In particular, the $\eta'$ interactions can be estimated from the large-$N_c$ effective...
Lagrangian, yielding interactions such as $n$-point $\eta'$ vertices which are suppressed at most by powers of $1/N_c$, but are otherwise of typical strong interaction size.

- The non-derivative couplings of the $\pi^0$ domain wall, which are suppressed by powers of the light quark masses (explicit chiral symmetry breaking) but which are still non-negligible. For example there are four $\pi$ interactions with coefficient $\sim \Sigma m/f_\pi^4$.

Due to the interactions mentioned above, the ADW will appear as a potential well of depth $\Lambda_{QCD}$ to the thermal hadrons at the QCD phase transition, which we expect to scatter with probability of order one. The ADW will contract at a rate \[ \frac{dE}{dt} \sim \sigma \frac{dl^2}{dt} \sim -\rho l^2 \] where $l$ is the size of the ADW, $\sigma \sim f_{PQ} f_\pi m_\pi$ is the surface tension of the domain wall and $\rho$ the hadron energy density. We will focus on the contribution to (21) from pions, because they are likely to have the highest energy density after the QCD phase transition. Since the quark condensate approaches zero at the chiral phase transition, we expect that the effective masses of the pions should be reduced. We therefore estimate the pion energy density to be given roughly by the standard relativistic formula for massless ($m << T$) particles

\[ \rho_\pi = \frac{\pi^2}{30} T^4 \sim f_\pi^4. \] (22)

This should be compared with the energy density of axions \[ \rho_a \sim 10^{-9} f_\pi^2 m_\pi^2. \] (23)

The contraction rate of the ADW from interactions with the $\pi$ and $\eta'$ thermal background is therefore very large

\[ \frac{dl}{dt} \sim \frac{f_\pi^2}{f_{PQ} l}. \] (24)

The rate of shrinkage in (24) is to be compared with the horizon doubling time $\sim M_P/f_\pi^2$. Since the Planck scale $M_P >> f_{PQ}$, we expect the ADW to contract away in a relatively short cosmological timescale, even if the effects of self-intersections are ignored.
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