QCD at Fixed Topology

R.Brower$^{a,b}$, S. Chandrasekharan$^{c,d}$, J. W. Negele$^b$ and U.-J. Wiese$^{b,d}$

$^a$ Department of Physics, Boston University
Boston, Massachusetts 02215, U.S.A.

$^b$ Center for Theoretical Physics,
Laboratory for Nuclear Science, and Department of Physics
Massachusetts Institute of Technology (MIT)
Cambridge, Massachusetts 02139, U.S.A.

$^c$ Department of Physics, Duke University
Durham, North Carolina 27708, U.S.A.

$^d$ Institute for Theoretical Physics, Bern University
3012 Bern, Switzerland

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Abstract

Since present Monte Carlo algorithms for lattice QCD may become trapped in a fixed topological charge sector, it is important to understand the effect of calculating at fixed topology. In this work, we show that although the restriction to a fixed topological sector becomes irrelevant in the infinite volume limit, it gives rise to characteristic finite size effects due to contributions from all $\theta$-vacua. We calculate these effects and show how to extract physical results from numerical data obtained at fixed topology.
1 Introduction

The numerical solution of lattice QCD is a notoriously hard problem. In particular, in order to obtain physical results, the numerical data must be extrapolated to the chiral, continuum, and infinite volume limits. Fortunately, the dependence of physical quantities on the quark masses, the lattice spacing, or the finite box size can often be understood analytically, and formulae can be derived that allow us to extrapolate reliably to the physical limit. Here we derive such formulae to correct for finite size effects that are due to fixed topology.

The configuration space of QCD decomposes into topological sectors. With boundary conditions that are periodic up to gauge transformations the topological charge $Q$ is an integer. In the continuum theory different topological sectors are separated by infinite action barriers. In a lattice theory the action barriers depend on the choice of the lattice action and the lattice definition of the topological charge. Although on the lattice the action barriers are typically finite, they may cause problems in the numerical sampling of the various $Q$ sectors. In particular, a standard algorithm (e.g. the hybrid Monte Carlo algorithm) that changes the gauge field configuration in small steps may get stuck in a fixed topological charge sector because it cannot overcome the action barriers. The question arises how one can extract meaningful physical information from numerical calculations that get stuck in a given topological sector. Locality and cluster decomposition properties suggest that the restriction to fixed topology becomes irrelevant in the infinite volume limit. Still, in order to extrapolate reliably to that limit, one must understand the corresponding finite size effects.

The Atiyah-Singer index theorem, $Q = n_L - n_R$, connects the physics of light quarks to the topology of the gluon field: the difference of the number of left- and right-handed zero modes of the Dirac operator, $n_L$ and $n_R$, is equal to the topological charge. Consequently, when one quark is exactly massless, the zero modes of the Dirac operator eliminate all nontrivial topological charge sectors (with $Q \neq 0$) from the QCD partition function. Hence, working at fixed $Q = 0$ is then correct even in a finite volume. However, even in that case various physical observables (e.g. the chiral condensate) get contributions from $Q \neq 0$ sectors, and one still needs to sample several topological sectors in order to compute those quantities. In the presence of a massless quark, the complex phase of the Boltzmann factor $\exp(i\theta Q)$ for a $\theta$-vacuum is trivial and the physics is independent of $\theta$. When all quarks are massive, there are nontrivial $\theta$-vacua effects and all topological sectors contribute to the partition function. In small space-time volumes with $\beta V \langle \bar{\Psi} \Psi \rangle m \ll 1$ (where $\beta$ is the inverse temperature, $V$ is the spatial volume, $\langle \bar{\Psi} \Psi \rangle$ is the chiral condensate, and $m$ is the quark mass) the partition function is still dominated by the $Q = 0$ contribution. On the other hand, in large volumes with $\beta V \langle \bar{\Psi} \Psi \rangle m \gg 1$ one must sample a large number of topological charge sectors.
When standard lattice fermion actions are used, the relation between the topology of the gluon field and the zero modes of the Dirac operator is obscured by lattice artifacts. In that case, the effects that we discuss here are difficult to observe in a numerical computation. However, when one uses a fermion action that obeys the Ginsparg-Wilson relation \cite{1}, the chiral properties of continuum fermions persist on the lattice. Our results — which we derive for the continuum theory — directly apply to this type of lattice fermions.

The rest of the paper is organized as follows. In section 2 the basic physics of $\theta$-vacua and the topological charge is reviewed, and in section 3 a simple formula for the fixed topology finite size effect on particle masses is derived. In section 4 chiral perturbation theory is used to study the $\theta$-dependence of the vacuum energy and the pion mass. In section 5, we explore the large $N_c$ limit in chiral perturbation theory. Since current lattice calculations are performed far from the chiral limit, in section 6 the $Q$-dependence of the $\eta'$-mass arising in an instanton gas model is estimated and compared with lattice results. Finally, section 7 contains the conclusions.

2 Topological Charge Sectors and $\theta$-Vacua

The partition function of QCD in a $\theta$-vacuum is given by

$$Z(\theta) = \int \mathcal{D}A \mathcal{D}\bar{\Psi} \mathcal{D}\Psi \exp(-S[A, \bar{\Psi}, \Psi]) \exp(-i\theta Q[A]),$$  \hspace{1cm} (2.1)

where

$$Q[A] = \frac{1}{32\pi^2} \int d^4x \, \epsilon_{\mu\nu\rho\sigma} \text{Tr} F_{\mu\nu} F_{\rho\sigma}$$  \hspace{1cm} (2.2)

is the topological charge of the gluon field $A_\mu(x) = iA_\mu^a(x)\lambda^a$ with field strength

$$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + [A_\mu(x), A_\nu(x)],$$  \hspace{1cm} (2.3)

and $S[A, \bar{\Psi}, \Psi]$ is the Euclidean QCD action, which is invariant under gauge transformations

$$A'_\mu(x) = g(x)(A_\mu(x) + \partial_\mu)g(x)^\dagger, \quad \Psi'(x) = g(x)\Psi(x), \quad \bar{\Psi}'(x) = \bar{\Psi}(x)g(x)^\dagger.$$  \hspace{1cm} (2.4)

We consider the theory in a finite spatial volume $V = L_x L_y L_z$ with periodic boundary conditions at temperature $T$, i.e. with finite Euclidean time extent $L_t = \beta = 1/T$. In order to allow for nontrivial topology, it is necessary to impose periodicity only for gauge invariant quantities. Thus, $A_\mu(x)$, $\Psi(x)$ and $\bar{\Psi}(x)$ are periodic only up to gauge transformations

$$A_\mu(x + L_\mu\hat{\mu}) = g_\mu(x)(A_\mu(x) + \partial_\mu)g_\mu(x)^\dagger, \quad \Psi(x + L_\mu\hat{\mu}) = g_\mu(x)\Psi(x), \quad \bar{\Psi}(x + L_\mu\hat{\mu}) = \bar{\Psi}(x)g_\mu(x)^\dagger.$$  \hspace{1cm} (2.5)
Here \( \hat{\mu} \) is the unit-vector in the \( \mu \)-direction and the \( g_\mu(x) \) are a set of transition functions that define the boundary condition. As first realized by 't Hooft \([2]\), for an \( SU(N_c) \) Yang-Mills theory these boundary conditions fall into gauge equivalence classes labeled by a twist tensor that takes values in the center of the gauge group. In general, for a nontrivial twist tensor, the topological charge can take fractional values that are multiples of \( 1/N_c \) \([3]\). In the presence of matter fields that transform nontrivially under the center (e.g. quarks in the fundamental representation of \( SU(3) \)), single valuedness of the matter field implies that the twist tensor is trivial. Hence, in the QCD case the topological charge is an integer and not a fraction. It is interesting to note that in supersymmetric Yang-Mills theory the gluinos, which transform under the adjoint representation, leave the center symmetry unbroken. Consequently, one then expects fractional topological charges. The role of the topological charge in QCD at finite volume has been worked out in great detail by Leutwyler and Smilga \([4]\). Although eq.(2.1) is quite formal, it can be given a concrete meaning on a space-time lattice using, for example, Ginsparg-Wilson fermions. Below we will ignore this subtlety and perform formal manipulations on eq.(2.1), assuming that all of these can be given a concrete realization on the lattice.

If we define \( H \) to be the QCD Hamiltonian with the energy eigenstates \( |n, \theta \rangle \) in a given \( \theta \)-vacuum, then we can write

\[
Z(\theta) = \sum_n \langle n, \theta | \exp(-\beta H) | n, \theta \rangle = \sum_n \exp(-\beta E_n(\theta)).
\]

(2.6)

For sufficiently large spatial volumes, the \( \theta \)-vacuum energy is given by \( E_0(\theta) = V e_0(\theta) \), where \( e_0(\theta) \) is the vacuum energy density. For small values of \( \theta \) it is given by

\[
e_0(\theta) = \frac{1}{2} \chi_t \theta^2 + \gamma \theta^4 + \ldots,
\]

(2.7)

where

\[
\chi_t = \frac{\langle Q^2 \rangle}{\beta V},
\]

(2.8)

is the topological susceptibility (at \( \theta = 0 \)). For \( \beta[E_1(\theta) - E_0(\theta)] \gg 1 \) the vacuum state dominates and we get

\[
Z(\theta) = \exp(-\beta V e_0(\theta)) = \exp(-\frac{\beta V \chi_t \theta^2}{2})[1 + O(\gamma \theta^4)].
\]

(2.9)

For small values of \( \theta \) and for \( M_\pi L \gg 1 \) (where \( L = L_x = L_y = L_z \) the first excited state is the pion, i.e. \( E_1 - E_0 = M_\pi \). On the other hand, in the limit of massless quarks chiral symmetry is restored in a finite volume and a rotor spectrum of states exists above the vacuum \([5]\). In that case, the energy of the first excited state is given by

\[
E_1(0) - E_0(0) = \frac{N_f^2 - 1}{N_f F_\pi^2 V},
\]

(2.10)

where \( N_f \) is the number of quark flavors and \( F_\pi \) is the pion decay constant. In other words, the energy gap is inversely proportional to the spatial volume. As the
quark mass increases, this state evolves into the state of a pion at rest. For \( \theta = \pi \) (depending on the quark masses and \( N_f \)) the CP symmetry breaks spontaneously \[6\]. In that case, there are two degenerate \( \theta \)-vacua in the infinite volume. In a finite volume, due to tunneling, there is an exponentially small energy gap

\[ E_1(\pi) - E_0(\pi) = A \exp(-\alpha V). \] (2.11)

Here \( \alpha \) is the tension of a 3-dimensional interface separating Euclidean space-time regions that are in distinct CP phases.

The QCD partition function at fixed topological charge \( Q \) is given by

\[ Z_Q = \int \mathcal{D}A \mathcal{D}\bar{\Psi} \mathcal{D}\Psi \, \delta_{Q,Q[A]} \exp(-S[A, \bar{\Psi}, \Psi]). \] (2.12)

Writing the Kronecker \( \delta \)-function as

\[ \delta_{Q,Q[A]} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, \exp[i\theta (Q - Q[A])], \] (2.13)

the fixed \( Q \) partition function turns into an integral over all \( \theta \) values

\[ Z_Q = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, Z(\theta) \exp(i\theta Q) \]
\[ = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \sum_n \exp(-\beta E_n(\theta)) \exp(i\theta Q). \] (2.14)

At sufficiently low temperatures (\( \beta E_1(0) \gg 1 \)) and sufficiently small topological charges (i.e. \( |Q|/\sqrt{\beta V} \) remains finite) the partition function reduces to

\[ Z_Q = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, \exp(-\beta V e_0(\theta)) \exp(i\theta Q). \] (2.15)

This equation is the starting point to derive the effects that we are interested in. For large space-time volumes \( \beta V \), the fixed \( Q \) partition function is dominated by the \( \theta \)-vacua with a small energy density. Since the \( \theta = 0 \) vacuum has the smallest energy, we see that the physics at large \( \beta V \) is dominated by \( \theta = 0 \). Hence, we can use a saddle point approximation to obtain a formula for \( Z_Q \). We assume a large \( \beta V \) keeping \( Q/\sqrt{\beta V} \) finite and fixed. Using eq.\(2.14\) one obtains

\[ Z_Q = \sqrt{\frac{2\pi}{\beta V \chi_t}} \exp\left[-\frac{Q^2}{2\beta V \chi_t}\right] \left\{ 1 + \mathcal{O}\left(\frac{\gamma}{\beta V}\right) \right\} \]
\[ = \sqrt{\frac{2\pi}{\langle Q^2 \rangle}} \exp\left[-\frac{Q^2}{2\langle Q^2 \rangle}\right] \left\{ 1 + \mathcal{O}\left(\frac{\gamma}{\beta V}\right) \right\}. \] (2.16)


3 Effective Mass Determination at fixed $Q$

It is possible to determine the hadron spectrum from a Monte Carlo simulation even if it gets stuck in a fixed topological sector. Typically hadron masses are extracted from 2-point correlation functions of operators with the appropriate quantum numbers. Higher $n$-point functions are important in the determination of other physical quantities like matrix elements and coupling constants. In a $\theta$-vacuum a general $n$-point correlation function of operators $\mathcal{O}_i$ takes the form

$$G(\theta) = \langle \mathcal{O}_1 \mathcal{O}_2 \ldots \mathcal{O}_n \rangle_{\theta} = \frac{1}{Z(\theta)} \int DAD\bar{\Psi}D\Psi \mathcal{O}_1 \mathcal{O}_2 \ldots \mathcal{O}_n \exp(-S[A, \bar{\Psi}, \Psi]) \exp(-i\theta Q[A]). \tag{3.1}$$

Hence, in a sector of fixed topological charge one obtains

$$G_Q = \langle \mathcal{O}_1 \mathcal{O}_2 \ldots \mathcal{O}_n \rangle_Q = \frac{1}{Z_Q} \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \ Z(\theta)G(\theta) \exp(i\theta Q). \tag{3.2}$$

Again, assuming small enough temperatures ($\beta E_1(0) \gg 1$) and sufficiently small topological charges (i.e. a finite $|Q|/\sqrt{\beta V}$), $Z_Q$ is given by eq.(2.16) and $Z(\theta)$ is given by eq.(2.9). Assuming that $\langle \mathcal{O}_1 \mathcal{O}_2 \ldots \mathcal{O}_n \rangle_{\theta}$ is smooth over the range $\theta^2 < 1/\beta V \chi_t = 1/\langle Q^2 \rangle$, one can again use the saddle point method to evaluate the integral over $\theta$. Then one obtains

$$G_Q = G(\theta_s) + \frac{1}{2\beta V \chi_t} G''(\theta_s) + \ldots, \tag{3.3}$$

where a prime denotes a derivative with respect to $\theta$. The (purely imaginary) value of $\theta$ at the saddle point is given by

$$\theta_s = i \frac{Q}{\beta V \chi_t} = i \frac{Q}{\langle Q^2 \rangle}. \tag{3.4}$$

Let us now consider a 2-point correlation function

$$\langle \mathcal{O}(t_1) \mathcal{O}(t_2) \rangle_{\theta}$$

$$= \frac{1}{Z(\theta)} \int DAD\bar{\Psi}D\Psi \mathcal{O}(t_1) \mathcal{O}(t_2) \exp(-S[A, \bar{\Psi}, \Psi]) \exp(-i\theta Q[A])$$

$$= \frac{1}{Z(\theta)} \sum_n \langle n, \theta | \mathcal{O}(-H(t_1 - t_2)) | \mathcal{O}(-H(\beta - t_1 + t_2)) | n, \theta \rangle$$

$$= \frac{1}{Z(\theta)} \sum_{m,n} \exp(-\beta E_m(\theta)) |\langle m, \theta | \mathcal{O} | n, \theta \rangle|^2 \exp[-(E_n(\theta) - E_m(\theta))(t_1 - t_2)], \tag{3.5}$$

relevant for determining particle masses. Here the operator $\mathcal{O}$ has the appropriate quantum numbers in order to create the particle of interest at rest from the $\theta = 0$
vacuum. The $\theta$-dependent particle mass is then given by $M(\theta) = E_1(\theta) - E_0(\theta)$. For large time separations ($t_1 - t_2$) and at sufficiently low temperatures (large $\beta$) the correlation function reduces to

$$\langle O(t_1)O(t_2) \rangle_\theta = |\langle 0, \theta|O|1, \theta \rangle|^2 \exp[-M(\theta)(t_1 - t_2)]. \quad (3.6)$$

Using eq.(3.3) and assuming

$$M(\theta) = M(0) + \frac{1}{2}M''(0)\theta^2 + \ldots, \quad (3.7)$$

one obtains

$$\langle O(t_1)O(t_2) \rangle_Q \sim A_Q \exp[-M_Q(t_1 - t_2)], \quad (3.8)$$

where $A_Q$ is a constant and

$$M_Q = M(0) + \frac{1}{2}M''(0)\frac{1}{\beta V \chi t} \left(1 - \frac{Q^2}{\beta V \chi t} \right) + \ldots \quad (3.9)$$

It should be noted that the concept of an effective “mass” $M_Q$ (which is independent of $t_1 - t_2$) in a fixed topological sector makes sense only to the quadratic order of the saddle point expansion considered here. Higher order terms lead to time-dependent “masses”. This is not surprising because, due to the topological constraint, QCD at fixed $Q$ is a nonlocal theory that does not even have a Hamiltonian. We note again that we take the large $\beta V$ limit keeping $Q/\sqrt{\beta V}$ fixed. Hence, the term $Q^2/\langle Q^2 \rangle$ is of order 1. When $Q$ itself is fixed this term becomes of order $1/\beta V$. In this case, there are other terms of the same order that we have not calculated. Hence, in order to be consistent, this term should then be dropped.

The above discussion shows that if a calculation performed in a space-time volume $\beta V$ gets stuck in a fixed $Q$ sector, one would extract a mass $M_Q$ that deviates from the infinite volume result by a term proportional to $1/(\beta V)$. This term decreases rapidly as one increases the space-time volume. Of course, from a simulation that is stuck in a fixed topological charge sector, one will not be able to extract $\langle Q^2 \rangle$, because it will be impossible to determine the relative weight of different sectors. Still, one should be able to perform separate computations for the various topological sectors, simply by starting the calculation in a given $Q$ sector. Then, in principle, one can measure $M_Q$ in the various sectors and at various space-time volumes and thereby extract $M(0)$, $M''(0)$ and $\langle Q^2 \rangle$ using eq.(3.9). It is interesting to note that when $M_Q$ is averaged over $Q$ with the distribution $\exp(-Q^2/2\langle Q^2 \rangle)$ one obtains the mass $M(0)$ in the $\theta = 0$ vacuum.

Let us briefly consider the extreme case of zero quark mass. Then the pion is massless and the box size is always small compared to the infinite Goldstone boson correlation length. For $m = 0$ there are no $\theta$-effects — $Z(\theta)$ is independent of $\theta$
— and the fixed $Q$ partition function $Z_Q$ is non-zero only for $Q = 0$. Hence, in this case, it is correct to work at fixed topological charge $Q = 0$, unless one wants to measure observables like the chiral condensate that receive contributions from $Q \neq 0$ sectors.

4 $\theta$-Dependence of Physical Quantities

Based on the previous discussion, it is clear that in a large space-time volume the effects of fixed topology can be determined from the $\theta$-dependence of certain physical quantities. For example, the partition function $Z_Q$ at fixed topological charge $Q$ can be determined from the $\theta$-dependence of the vacuum energy $e_0(\theta)$ using eq. (2.15) and the effective mass of a hadron $M_Q$ can be obtained from $M(\theta)$ using eq. (3.9).

Until now we have written the QCD action in a $\theta$-vacuum as $S[A, \Psi, \bar{\Psi}] + i\theta Q[A]$. It is well known that, using an anomalous $U(1)_A$ chiral transformation, the $\theta$-dependence can be moved into the quark mass matrix $\mathcal{M} = \text{diag}(m_u, m_d, ..., m_{N_f})$ (for $N_f$ flavors), i.e.

$$S_\theta[A, \Psi, \bar{\Psi}] = \frac{1}{g^2} \int d^4x \, \text{Tr} F_{\mu\nu} F_{\mu\nu} + \int d^4x \, \left\{ \bar{\Psi}_L \gamma_\mu (A_\mu + \partial_\mu) \Psi_L + \bar{\Psi}_R \gamma_\mu (A_\mu + \partial_\mu) \Psi_R \right\} + \int d^4x \, \left\{ \bar{\Psi}_L \mathcal{M} e^{i\theta/N_f} \Psi_R + \bar{\Psi}_R \mathcal{M}^\dagger e^{-i\theta/N_f} \Psi_L \right\}.$$  (4.1)

Thus, $\theta$ appears simply as the complex phase of the determinant of the mass matrix.

Although $\theta$ enters the QCD action in a simple way, in general its effects on physical quantities are difficult to determine. However, for small quark masses chiral perturbation theory allows us to understand such effects. It is well known that the low-energy physics of Goldstone bosons in QCD can be described systematically using an effective theory. In the case of $N_f$ light quarks to lowest order the action of the Goldstone boson field $U \in SU(N_f)$ takes the form

$$S[U] = \int d^4x \left\{ \frac{F_\pi^2}{4} \text{Tr}[\partial_\mu U^\dagger \partial_\mu U] - \frac{1}{2N_f} \text{Tr}[\mathcal{M} e^{i\theta/N_f} U^\dagger + \mathcal{M}^\dagger e^{-i\theta/N_f} U] \right\},$$  (4.2)

where $F_\pi$ is the pion decay constant. The term proportional to $F_\pi^2$ is invariant under chiral $SU(N_f)_L \otimes SU(N_f)_R$ transformations

$$U'(x) = LU(x)R^\dagger,$$  (4.3)

(with $L \in SU(N_f)_L$ and $R \in SU(N_f)_R$) while the mass term explicitly breaks chiral symmetry.
First, we consider the case of $N_f$ degenerate flavors of mass $m$. Then the mass matrix takes the form $M = m 1$. In this case, the chiral symmetry is explicitly broken down to the vector subgroup $SU(N_f)_{L=R}$. When the vacuum angle changes by $2\pi n$, exp$(i\theta/N_f)$ changes by an element $z = \exp(2\pi n i/N_f) \in Z(N_f)$ — the center of the flavor group $SU(N_f)$. Although the action itself is not $2\pi$-periodic in $\theta$, the corresponding partition function

$$Z(\theta) = \int D U \ \exp(-S[U])$$

is, because the shift exp$(i\theta'/N_f) = z \exp(i\theta/N_f)$ can be compensated by a redefinition of the field $U' = z U$. For $\theta \in [-\pi, \pi]$, the effective action is minimized by constant field configurations $U = 1$. The value of the action at the minimum

$$S[1] = -\beta V \langle \bar{\Psi} \Psi \rangle m \cos(\theta/N_f)$$

determines the $\theta$-vacuum energy density (normalized to zero at $\theta = 0$) as

$$e_0(\theta) = \langle \bar{\Psi} \Psi \rangle m (1 - \cos(\theta/N_f)).$$

This expression is valid for $\theta \in [-2\pi/N_f, 2\pi/N_f]$. When extended periodically to other $\theta$-values, it has cusps at $\theta = 4\pi (n + 1/2)/N_f$ indicating a phase transition in the vacuum angle [6]. Comparing this result with eq.(2.7), we identify the topological susceptibility as

$$\chi_t = \langle \bar{\Psi} \Psi \rangle m N_f^2 / F^2 \pi.$$  

In order to determine the $\theta$-dependence of the Goldstone boson mass, we expand $U = \exp(i\pi^a \lambda^a / F^2 \pi)$ in powers of $\pi^a$ and read off $M^2_\pi(\theta)$ as the coefficient of the $\pi^a \pi^a$ term. This yields

$$M^2_\pi(\theta) = M^2_\pi(0) \cos(\theta/N_f),$$

where

$$M^2_\pi(0) = 2m \langle \bar{\Psi} \Psi \rangle N_f F^2 \pi / F^2 \pi,$$

is the Goldstone boson mass squared at $\theta = 0$.

Using leading order baryon chiral perturbation theory [7] the quark mass dependence of the nucleon mass (at $\theta = 0$) is given by

$$M_N(0) = M_N^0 [1 + c \frac{M^2_\pi}{F^2 \pi}] - \frac{3g_A^2 M^2_\pi}{32\pi F^2 \pi},$$

where $M_N^0$ and $g_A$ are the nucleon mass and the neutron decay constant in the chiral limit, and $c$ is a known combination of low-energy constants. At this order in chiral perturbation theory the $\theta$-dependence enters only through the pion mass of eq.(4.8) such that

$$M_N(0) = M_N^0 [1 + c \frac{M^2_\pi \cos(\theta/N_f)}{F^2 \pi}] - \frac{3g_A^2 M^3_\pi \cos^3/2(\theta/N_f)}{32\pi F^2 \pi},$$
Let us now consider the case of two non-degenerate flavors with masses \( m_u \) and \( m_d \). Then the mass matrix takes the form \( \mathcal{M} = \text{diag}(m_u, m_d) \), and chiral symmetry is explicitly broken down to \( U(1)_{L=R} \). Now the action is minimized for \( U = \text{diag}(\exp(i\varphi), \exp(-i\varphi)) \) where

\[
\tan \varphi = \frac{m_u - m_d}{m_u + m_d} \tan \frac{\theta}{2},
\]

and one obtains

\[
e_0(\theta) = \langle \bar{\Psi}\Psi \rangle \frac{m_u + m_d}{2} \left[ 1 - \cos \left( \frac{\theta}{2} \right) \sqrt{1 + \frac{(m_u - m_d)^2}{(m_u + m_d)^2} \tan^2 \frac{\theta}{2}} \right].
\]

The pion mass is given by

\[
M_{\pi}^2(\theta) = M_{\pi}^2(0) \cos \left( \frac{\theta}{2} \right) \sqrt{1 + \frac{(m_u - m_d)^2}{(m_u + m_d)^2} \tan^2 \frac{\theta}{2}},
\]

where now

\[
M_{\pi}^2(0) = \left. \langle \bar{\Psi}\Psi \rangle (m_u + m_d) \right/ 2 F_{\pi}^2.
\]

### 5 \( \theta \)-Dependence at large \( N_c \)

The flavor-singlet pseudoscalar particle \( \eta' \) is special in QCD. Due to the anomaly it is heavy (and thus not a Goldstone boson) and hence its physics cannot be understood using chiral perturbation theory. However, in the large \( N_c \) limit the anomaly disappears and the \( \eta' \) becomes a Goldstone boson which can now be studied in chiral perturbation theory. The low-energy effective action of eq.(4.2) is modified to

\[
S[U] = \int d^4x \left\{ \frac{F_{\pi}^2}{4} \text{Tr}[\partial_{\mu} \tilde{U}^{\dagger} \partial_{\mu} \tilde{U}] - \frac{\langle \bar{\Psi}\Psi \rangle}{2N_f} \text{Tr}[\mathcal{M} \epsilon^{i\theta/N_f} \tilde{U}^{\dagger} + \mathcal{M}^{\dagger} e^{-i\theta/N_f} \tilde{U}] \right\}
+ \frac{1}{2} \lambda_0^0 (i \log \det \tilde{U})^2.
\]

Here \( \tilde{U} \) is a \( U(N_f) \) matrix with complex determinant \( \exp(i \sqrt{2N_f \eta' / F_{\pi}}) \). The last term in eq.(5.1) gives rise to the \( \eta' \) mass

\[
M_{\eta'}^2 = \frac{2N_f \lambda_0^0}{F_{\pi}^2}.
\]

At large \( N_c \) the pion decay constant goes as \( F_{\pi}^2 \sim N_c \) while the topological susceptibility \( \chi_t^0 \) of the quenched (zero flavor) theory is of order 1. Hence, as \( N_c \) goes to infinity, the \( \eta' \)-meson becomes a massless Goldstone boson. The occurrence of the
\( \eta' \) field in the chiral Lagrangian has a dramatic effect on the \( \theta \)-dependence. Since \( \theta \) enters as the determinant of the mass matrix, it can be absorbed into a redefinition of the field \( \eta' \) such that

\[
S[\tilde{U}] = \int d^4x \left\{ \frac{F^2}{4} \text{Tr}[\partial_\mu \tilde{U}^\dagger \partial_\mu \tilde{U}] - \frac{\langle \bar{\Psi} \Psi \rangle}{2N_f} \text{Tr}[\mathcal{M} \tilde{U}^\dagger + \mathcal{M}^\dagger \tilde{U}] \right\} + \frac{1}{2} \chi^0_i (i \log \det \tilde{U} - \theta)^2.
\] (5.3)

At large \( N_c \) the last term in eq.(5.3) can be neglected and thus all \( \theta \)-dependence disappears from the theory even at non-zero quark masses. This is consistent because the anomaly disappears in the large \( N_c \) limit and \( U_A(1) \) chiral rotations can be used to relate different \( \theta \)-vacua which thus become physically indistinguishable.

At large but finite \( N_c \) we can use the action of eq.(5.3) to derive the \( \theta \)-dependence of the Goldstone boson masses for \( N_f \) degenerate quark flavors of mass \( m \). First, we must find the minimum of the action, which turns out to be at

\[
\tilde{U} = \exp(i \sqrt{2/N_f} \eta'_0(\theta)/F_\pi) \mathbb{1},
\] (5.4)

where

\[
\langle \bar{\Psi} \Psi \rangle m \sin \left( \sqrt{\frac{2}{N_f}} \frac{\eta'_0(\theta)}{F_\pi} \right) + \chi^0_i N_f (\sqrt{2N_f} \frac{\eta'_0(\theta)}{F_\pi} - \theta) = 0.
\] (5.5)

When one is closer to the chiral than to the large \( N_c \) limit the second term on the left-hand side of eq.(5.5) dominates and then

\[
\eta'_0 = \frac{F_\pi}{\sqrt{2N_f}} \theta.
\] (5.6)

It is easy to show that the vacuum energy takes the form

\[
e_0(\theta) = -m \langle \bar{\Psi} \Psi \rangle \cos \left( \sqrt{\frac{2}{N_f}} \frac{\eta'_0(\theta)}{F_\pi} \right) + \frac{1}{2} \chi^0_i \left( \sqrt{2N_f} \frac{\eta'_0(\theta)}{F_\pi} - \theta \right)^2.
\] (5.7)

The \( \theta \)-dependence of the pion mass

\[
M^2_\pi(\theta) = M^2_\pi(0) \cos \left( \sqrt{\frac{2}{N_f}} \frac{\eta'_0(\theta)}{F_\pi} \right),
\] (5.8)

is similar to the one in eq.(4.8) except that \( \theta \) is now replaced by \( \sqrt{2N_f} \eta'_0(\theta)/F_\pi \). The \( \eta' \) mass is given by

\[
M^2_{\eta'}(\theta) = 2N_f \chi^0_i \frac{F_\pi^2}{F_\pi^2} + M^2_\pi(\theta).
\] (5.9)

At \( N_c = \infty \) the first term on the right-hand side of eq.(5.9) vanishes, thus making \( \eta' \) degenerate with the pion. Solving explicitly for \( \eta'_0 \), we also note that in the limits \( m \to 0 \) or \( N_c \to \infty \) physical quantities become \( \theta \)-independent.
Recently, the dependence of $M_\pi$ and $M_{\eta'}$ on $Q$ has been studied in lattice calculations [8]. Each mass was evaluated in two domains, one with $|Q| \leq 1$ and the other with $|Q| \geq 2$. While the pion masses in both domains agreed with each other within statistical errors of a few percent, the $\eta'$-mass was about 15 percent heavier in the $|Q| \geq 2$ domain than in the $|Q| \leq 1$ domain. Unfortunately, the quark masses used in current lattice calculations are far from the chiral limit such that the above results from chiral perturbation theory should not be applicable to these lattice data. For example, in a typical full QCD lattice calculation $M_\pi/M_\rho \geq 0.6$. Still, it is tempting to compare our predictions with the lattice data. Assuming that we are closer to the chiral than to the large $N_c$ limit, using eqs. (5.5, 5.9) we find

$$M_{\pi Q} = M_\pi(0) \left[ 1 - \frac{1}{4 N_f^2} \frac{1}{\langle Q^2 \rangle} \left( 1 - \frac{Q^2}{\langle Q^2 \rangle} \right) \right].$$

(5.10)

In the lattice calculation of [8] $\beta V = 6.81 \text{fm}^4$, $\chi_t = 0.70 \text{fm}^{-4}$, and hence $\langle Q^2 \rangle = \beta V \chi_t = 4.75$. This means that the predicted shift of the effective pion mass at $Q = 0$ is given by $-M_\pi(0)/(4 N_f^2 \langle Q^2 \rangle) = 0.013 M_\pi(0)$. Hence, the effect of fixed topology is of the order of 1 percent, consistent with the lattice results.

At large but finite $N_c$ and close enough to the chiral limit (i.e. when eqs. (5.8, 5.9) apply) the second $\theta$-derivatives $M_{\eta'}''(0)$ and $M_\pi''(0)$ are equal. Hence, using eq. (3.9) we would expect that the $Q$-dependent shift of the effective masses of $\eta'$ and the pion are the same, in disagreement with the lattice results.

### 6 Q-Dependence in an Instanton Gas

It is useful to try to understand how fixed topology affects QCD in the domain explored by actual lattice calculations. Motivated by the phenomenological success of the Veneziano-Witten formula [9, 10] relating the $\eta'$-mass to the quenched topological susceptibility $\chi_t^0$, in this section we will seek a qualitative understanding of the $Q$-dependence of the $\eta'$-mass by modeling the fluctuations of the topological charge by an instanton gas.

We begin by assuming independent Poisson distributions for instantons and anti-instantons in a space-time volume $\beta V$ with $\langle N \rangle = \langle \bar{N} \rangle = \lambda$. Then the probability of having $N$ instantons and $\bar{N}$ anti-instantons is given by

$$P(N, \bar{N}) = \frac{\lambda^{(N+\bar{N})}}{N! \bar{N}!} e^{-2\lambda}. \quad (6.1)$$

Using $Q = N - \bar{N}$ one obtains

$$\langle Q^2 \rangle = \langle N + \bar{N} \rangle = 2\lambda = \beta V \chi_t^0. \quad (6.2)$$
Fixing the topological charge to $Q$ the probability distribution takes the form
\[ P_Q(N, \bar{N}) = \frac{1}{Z_Q} \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \frac{\lambda^{N+\bar{N}}}{N!\bar{N}!} e^{-2\lambda \exp[i\theta(Q - (N - \bar{N})]}. \tag{6.3} \]

where
\[ Z_Q = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \exp[-2\lambda(1 - \cos \theta)] \exp(i\theta Q). \tag{6.4} \]

Motivated by eq. (6.2) we want to model the $Q$-dependence of the $\eta'$-mass by assuming
\[ M_{\eta'Q}^2 = \frac{2N_f}{F_\pi^2} \frac{\langle N + \bar{N}\rangle_Q}{\beta V}. \tag{6.5} \]

In the large $\beta V$ limit (with $Q/\sqrt{\beta V}$ fixed) one obtains
\[ \frac{\langle N + \bar{N}\rangle_Q}{\beta V} = \chi_T^0 - \frac{1}{2\beta V} \left[ 1 - \frac{Q^2}{\beta V \chi_T^0} \right]. \tag{6.6} \]

This is a simple and physically appealing result. When $M_{\eta'Q}^2$ is averaged with the distribution $Z_Q \sim \exp(-Q^2/2\langle Q^2 \rangle)$ in the appropriate limit, the $\eta'$ mass is consistent with the Veneziano-Witten formula. The finite volume corrections provide the desired $Q$-dependence. Using eqs. (6.5, 6.6) for $M_{\eta'Q}^2$, we find that the percentage shift of $M_{\eta'}$ at $Q = 0$ is given by $1/4\beta V \chi_T^0 = 1/4\langle Q^2 \rangle$. In the lattice calculation of $\chi_T^0 = 0.06$, which is of the same order of magnitude as the observed 10 percent shift in the $\eta'$-mass between the sum over all $Q$ and the sum over $|Q| < 1.5$.

7 Conclusions

In this work, we have shown how to correct finite size effects that occur in lattice QCD calculations at fixed topology. We have derived a formula that relates the $Q$-dependent effective mass $M_Q$ to the true mass $M(0)$ and its second derivative $M''(0)$ at vacuum angle $\theta = 0$. The difference $M_Q - M(0)$ is of the order $1/\beta V$ and thus vanishes quickly in the large volume limit. By observing the predicted finite size effect in a lattice calculation that gets stuck in fixed topological charge sector, one can identify not only $M(0)$ but also $M''(0)$ and thus one can learn something about the $\theta$-dependence. Close to the chiral limit, we have used chiral perturbation theory to predict $M''(0)$ for the pion and the nucleon. For large $N_c$ we have also derived this quantity for the $\eta'$-meson. Our formulae are in reasonable agreement with existing lattice data for the effective pion mass at fixed $Q$, despite the fact that those calculations are performed far from the chiral limit. On the other hand, perhaps not surprisingly, the observed $Q$-dependent effective $\eta'$-mass does not agree with the large $N_c$ chiral prediction. Interestingly, a dilute instanton gas model is qualitatively consistent with the lattice data.
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