Physical Observables from Lattice QCD at Fixed Topology

R. Brower a, S. Chandrasekharan b J. W. Negele c and U.-J. Wiese c†

aDepartment of Physics, Boston University, Boston, Massachusetts 02215, USA
bDepartment of Physics, Duke University, Durham, North Carolina 27708, USA
cCenter for Theoretical Physics, MIT, 77 Massachusetts Ave., Cambridge, MA 02139, USA

Because present Monte Carlo algorithms for lattice QCD may become trapped in a given topological charge sector when one approaches the continuum limit, 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. TOPOLOGICAL CHARGE SECTORS AND \(\theta\)-VACUA

In principle, one should calculate observables in QCD with finite quark masses in a fixed \(\theta\)-vacuum. However in practical lattice calculations, algorithms that change the gauge field configuration in small steps tend to become trapped in a fixed topological charge sector because they cannot overcome the action barriers between sectors. One sees concrete evidence of this problem, for example, from the large equilibration times for the topological charge required in hybrid Monte Carlo calculations, which increase as the quark mass is decreased [1]. In addition, improved pure gauge actions, such as DBW2, reduce the low eigenmodes that are undesirable for overlap and domain wall fermions by suppressing small instantons and thereby reduce tunneling between sectors. Since we know that the restriction to fixed topology becomes irrelevant in the infinite volume limit, we have calculated the finite volume dependence of this restriction and thereby show how to extract physical results from practical calculations at fixed topology.

The partition function of the QCD Hamiltonian \(H\) with eigenstates \(|n, \theta\rangle\) in a given sector may be written in terms of the lowest eigenvalue \(E_0(\theta) = Ve_0(\theta)\) in the large volume, low temperature limit as follows:

\[
Z_\theta = \text{Tr}_\theta e^{-\beta H} = \sum_n e^{-\beta E_n(\theta)} \rightarrow e^{-\beta Ve_0(\theta)}.
\]

The partition function at fixed topological charge \(Q\) is an integral over all \(\theta\)-vacuum sectors. Expanding the ground state energy

\[
e_0(\theta) = e_0(0) + \frac{1}{2} \chi_t \theta^2 + \frac{1}{24} \gamma \theta^4 + ...,
\]

and performing a saddle-point expansion to \(\mathcal{O}(1/\beta^2 V^2)\),

\[
Z_Q = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \ Z_\theta e^{i\theta Q} \
\rightarrow \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \ e^{i\theta Q} e^{-\beta Ve_0(\theta)} \ 
\simeq \ e^{-\beta Ve_0(0)} \sqrt{\frac{2\pi}{\beta V \chi_t}} \ e^{-\frac{\theta^2}{2\chi_t}} \ 
\times \left[ 1 - \frac{\gamma}{24\beta V \chi_t} \left( 3 - \frac{6}{\chi_t} Q^2 + \frac{1}{\chi_t^2} \frac{Q^4}{\beta^2 V^2} \right) \right].
\]

Using \(Z_\theta = \int DAD\bar{\Psi}D\Psi \ e^{-S[A,\bar{\Psi},\Psi]-i\theta Q[A]}\), the parameters in the expansion of \(e_0(\theta)\) are

\[
\chi_t = \frac{\langle Q^2 \rangle}{\beta V}, \quad \gamma = -\frac{\langle Q^4 \rangle - 3\langle Q^2 \rangle^2}{\beta V}. \quad (2)
\]
The topological susceptibility, $\chi_t$, and fourth moment, $\gamma$, are parameters characterizing the vacuum that can be calculated in lattice QCD. Once they are known, we may use eq. (3) to calculate any observable at fixed $Q$ and obtain finite volume corrections.

2. MASS SPECTRUM IN A FIXED TOPOLOGICAL SECTOR

As a concrete example, consider the calculation of hadron masses from the large time behavior of two-point correlation functions. At sufficiently low temperature, the two-point correlation function at fixed $Q$ of operators $\mathcal{O}$ with the appropriate quantum numbers to create the hadron states of interest may be written

\[
\langle \mathcal{O}(t_1)\mathcal{O}(t_2) \rangle_Q = \frac{1}{Z_Q} \int_{-\pi}^{\pi} d\theta e^{iQ\theta - \beta V c_{\epsilon} (\theta)} \times |\langle 0, \theta | \mathcal{O}[1, \theta] \rangle|^2 e^{-M(\theta)(t_1 - t_2)},
\]

where $M(\theta)$ is the lowest hadron mass. Performing a saddle-point expansion, the effective mass used to measure the hadron spectrum is

\[
M_Q^{eff} = -\frac{d}{dt_1} \log(\langle \mathcal{O}(t_1)\mathcal{O}(t_2) \rangle_Q) = \frac{1}{\beta V} \int_{-\pi}^{\pi} d\theta e^{-\frac{1}{2}Q^2\theta^2 + i\theta Q f(\theta) M(\theta)} f(\theta) \, d\theta,
\]

where $f(\theta) = |\langle 0, \theta | \mathcal{O}[1, \theta] \rangle|^2 e^{-M(\theta)(t_1 - t_2)}$ contains all the time dependence. Expanding $M(\theta) = M(0) + \frac{1}{2} M''(0) \theta^2 + \frac{1}{4} M'''(0) \theta^4 + \cdots$ and $f(\theta) = f(0) + \frac{1}{2} f''(0) \theta^2 + \frac{1}{4} f'''(0) \theta^4 + \cdots$ we obtain the desired expansion,

\[
M_Q^{eff} = M(0) + \frac{1}{2} M''(0) \, \overline{\theta}^2 + \frac{1}{4!} M'''(0) \, \overline{\theta}^4 + \frac{6}{4!} f''(0) M''(0) \, \overline{\theta}^4 + \cdots
\]

where

\[
\overline{\theta} = \frac{\int d\theta \exp(-\frac{1}{2}(Q^2)\theta^2 + iQ\theta) \theta^n}{\int d\theta \exp(-\frac{1}{2}(Q^2)\theta^2 + iQ\theta)}.
\]

The moments required in eq. (3) are

\[
\overline{\theta}^2 = \frac{1}{(Q^2)^2} \left( 1 - \frac{Q^2}{(Q^2)^2} \right),
\]

\[
\overline{\theta}^4 = \frac{1}{(Q^2)^2} \left( 3 - \frac{6 Q^2}{(Q^2)^2} + \frac{Q^4}{(Q^2)^2} \right),
\]

where $\langle Q^2 \rangle = \beta V \chi_t$ by eq. (3). Note that to leading order, all dependence of the mass shift on $f(\theta)$ exactly cancels and therefore the result is independent of $t_1 - t_2$.

Our leading order result for the $Q$-dependence of the mass is thus

\[
M_Q^{eff} = M(0) + \frac{1}{2} M''(0) \left( 1 - \frac{Q^2}{\beta V \chi_t} \right).
\]

Therefore, if a calculation in a volume $\beta V$ is trapped in a $Q$ sector, the error is of order $1/(\beta V)$. Furthermore, one can measure $M_Q$ in several sectors and at several space-time volumes and thereby extract $M(0)$, $M''(0)$, and $\chi_t$ using eq. (3). Also note that when averaged over $Q$ with the distribution $e^{-\frac{Q^2}{\beta V}}$, $\langle \overline{\theta}^2 \rangle = 0$.

3. $\theta$ DEPENDENCE IN THE CHIRAL AND LARGE $N_c$ LIMITS

It is possible to make some general arguments concerning the $\theta$-dependence in QCD. The transformation $\psi' = \exp(i \frac{\theta}{2\pi} \gamma_5) \psi$ shifts the $\theta$-dependence to the mass term,

\[
m\overline{\Psi} \Psi \rightarrow \overline{n} \{ m \cos(\theta/N_f) + im \sin(\theta/N_f) \gamma_5 \} \Psi
\]

and the contribution to the fermionic measure cancels the $F\overline{F}$-term. By parity, the $\sin(\theta/N_f)$ term only contributes in even orders, so at linear order in the quark mass, the only effect of $\theta$ enters through the change of the mass term to $m \cos(\theta/N_f)$. Hence, for example, to leading order in the chiral limit, the pion, nucleon and $\eta'$ masses must have the forms:

\[
M_\pi^2(\theta) = M_\pi^2(0) + M_\pi^2(0) \sin^2(\theta/N_f) - 1
\]

\[
M_N(\theta) = M_N(0) + c_1 M_N^2(0) \sin^2(\theta/N_f) - 1
\]

\[
M_{\eta'}^2(\theta) = M_{\eta'}^2(0) + b_1 M_{\eta'}^2(0) \sin^2(\theta/N_f) - 1
\]

from which the $Q$-dependence follows directly from eq. (3). In the large $N_c$ limit, it can be shown that $b_1 = 1$ so that the $\pi$ and $\eta'$ have the same $\theta$-dependence and thus the same $Q$-dependence.

Using chiral perturbation theory, one can explore the chiral and large $N_c$ limits more systematically. Using the effective Lagrangian proposed...
by Witten [2] to treat the $U_A(1)$ anomaly, we obtain the following results for the $\pi$ and $\eta'$ masses:

\[ M_{\pi}^2 = \frac{2m\langle\bar{\Psi}\Psi\rangle}{N_f F_\pi^2} \cos \left( \frac{\eta_0}{F_\pi} \sqrt{\frac{2}{N_f}} - \frac{\theta}{N_f} \right) \]

\[ M_{\eta'}^2 = m_0^2 + \frac{2m\langle\bar{\Psi}\Psi\rangle}{N_f F_\pi^2} \cos \left( \frac{\eta_0}{F_\pi} \sqrt{\frac{2}{N_f}} - \frac{\theta}{N_f} \right) \]

where \( c_0(\theta) = -m\langle\bar{\Psi}\Psi\rangle \cos \left( \frac{\eta_0}{F_\pi} \sqrt{\frac{2}{N_f}} - \frac{\theta}{N_f} \right) + \frac{m_0^2}{2N_c} \eta'^2 \).

Solving explicitly for $\eta_0$, we also note that in the limit $m \to 0$, we recover cos $\left( \frac{m_0^2 F_\pi^2 \theta}{2m\langle\bar{\Psi}\Psi\rangle N_c} \right) \to 1$ as $N_c \to \infty$ we obtain cos $\left( \frac{m_0^2 F_\pi^2 \theta}{2m\langle\bar{\Psi}\Psi\rangle N_c} \right) \to 1$ as $N_c \to \infty$ as expected.

4. Q – DEPENDENCE IN AN INSTANTON GAS

Recently, the dependence of the $\pi$ and $\eta'$ masses on $Q$ has been studied in lattice calculations [3], which for practical reasons, are sufficiently far from the chiral limit that the previous results from chiral perturbation theory are inapplicable. Each mass was evaluated in two sectors, one with $|Q| < 1.5$ and the other with $|Q| > 1.5$. Whereas the pion mass in both sectors agreed within statistics of a few percent, the $\eta'$ mass was of the order of 15% heavier in the $|Q| > 1.5$ sector than in the $|Q| < 1.5$ sector. Motivated by the success of the Veneziano-Witten formula [3] [4] relating the $\eta'$ mass to fluctuations in the topological charge, we obtain a qualitative understanding of the $Q$ dependence from the fluctuations in the topological charge arising in an instanton gas.

The vertex generating the shift in the $\eta'$ mass is proportional to the number of instantons, $N$, plus the number of antiinstantons, $\bar{N}$. Assuming independent Poisson distributions with $\langle N \rangle = \langle \bar{N} \rangle = \lambda$, the probability of having $N$ instantons and $\bar{N}$ antiinstantons with the constraint $N - \bar{N} = Q$ is:

\[ P_Q(N, \bar{N}) = \int \frac{d\theta}{2\pi} \frac{\lambda^{(N+\bar{N})}}{N!\bar{N}!} e^{-2\lambda - i\theta(Q-N+\bar{N})} \]

Summing over $N$ and $\bar{N}$ and distinguishing $\lambda$ and $\lambda'$ for subsequent convenience, we write the generating function

\[ Z_Q(\lambda, \lambda') = \sum_{N, \bar{N}} \int \frac{d\theta}{2\pi} \frac{\lambda^{(N+\bar{N})}}{N!\bar{N}!} e^{-2\lambda - i\theta(Q-N+\bar{N})} \]

\[ = e^{-2\lambda} \int \frac{d\theta}{2\pi} e^{-i\theta Q + 2\lambda' \cos(\theta)} \]

\[ \approx \frac{1}{2\sqrt{\pi \lambda'}} e^{2(\lambda'-\lambda)} e^{-\frac{Q^2}{4\lambda'}} \]

Differentiation of $\ln Z_Q(\lambda, \lambda')$ with respect to $\lambda'$, setting $\lambda = \lambda'$, and noting $2\lambda = \langle Q^2 \rangle = \chi_0 \beta V$ yields the desired result for the density of instantons plus antiinstantons at fixed $Q$:

\[ \frac{\langle N + \bar{N} \rangle_Q}{\beta V} = \chi_0 + \frac{1}{2\beta V} \left[ -1 + \frac{Q^2}{\chi_0 \beta V} \right] \]

Eq. [3] is a simple and physically appealing result. Since $M_{\eta'}^2 = M_{\eta}^2 + \mu$ and $\mu \propto \frac{\langle N + \bar{N} \rangle}{2\beta V}$, which equals $\chi_0$ when averaged over the distribution $P(Q) = \frac{1}{2\sqrt{\pi \lambda'}} e^{-\frac{Q^2}{4\lambda'}}$, the $\eta'$ mass is consistent with the Veneziano-Witten formula. The finite volume corrections provide the desired $Q$ dependence.

To compare with the lattice results of ref [3], we note that $\beta V = 6.81 fm^4$, $\chi_0 = 0.70 fm^{-4}$, and $\langle Q^2 \rangle = 4.75$. In the chiral limit, $M_{\eta}^{eff}(Q) = M_{\pi}(0) - M_{\pi} \left( \frac{1}{4N_f} \left( 1 - \frac{Q^2}{(Q^2)} \right) \right)$, so the shift at $Q^2 = 0$ is $-M_{\pi}/(4N_f^{\langle Q^2 \rangle} = 0.013 M_{\pi}$. Hence, the effect of calculation at fixed topology is of the order of 1%, consistent with the lattice $\pi$ results. The analogous chiral estimate for the $\eta'$ is of order $(M_{\pi}/M_{\eta'})^2 \times 1\%$, in strong disagreement with lattice results. However, using the instanton gas result, $\int dq P(Q) (\frac{N+\bar{N}}{2\beta V})^2$ is $0.65$ for $Q < 1.5$ and $0.75$ for $Q > 1.5$, yielding $\delta M_{\eta'}/M_{\eta'} = 8\%$, which is of the order of magnitude of the observed $Q$ dependence.

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