Screening of the topological charge in a correlated instanton vacuum

E.V. Shuryak and J.J.M. Verbaarschot

Department of Physics
SUNY, Stony Brook, New York 11794

Abstract

Screening of the topological charge due to fermion-induced interactions is an important phenomenon, closely related with the resolution of the strong CP and U(1) problems. We study the mechanism of such screening in a 'correlated instanton vacuum', as opposed to the 'random' one. Both scalar and pseudoscalar gluonic correlators are analyzed by means of an observable that minimizes finite size effects. Screening of the topological charge is established. This allows us to calculate the $\eta'$ mass without having to invert the Dirac operator. We suggest that this method might be used in lattice QCD calculations as well. Our results for the screening of the topological charge are in agreement with the chiral Ward identities, and the scalar gluonic correlator satisfies a low energy theorem first derived by Novikov et al. [1]. We also propose to evaluate the topological susceptibility in the Witten-Veneziano formula not in an infinite box in a world \textit{without} fermions but in an infinitesimal box in a world \textit{with} fermions.
1 Introduction

Tunneling between topologically distinct sectors of the gauge field, which is described semiclassically by instantons [2, 3], is known to be one of the major non-perturbative phenomena in QCD. Their importance was significantly clarified in the last few years. In particular, a large set of QCD correlation functions was studied [4, 5, 6] in the so called 'random instanton liquid model', RILM. The results are in surprisingly good agreement both with experiment (see [7]) and lattice data [8]. They clearly show that many hadrons (including e.g. pions and nucleons) are actually bound by the instanton-induced interactions, and their properties such as masses (and even wave functions [9]) can be well reproduced by the simplest instanton-based model.

Secondly, important new results were obtained from the study of 'cooled' lattice configurations. ('Cooling' is a procedure that relaxes any given gauge field configuration to the closest 'classical component' of the QCD vacuum.) Not only were they found to be of the multi-instanton type [10], but recent work of Chu et al. [11] has essentially reproduced the key parameters of the 'instanton liquid' picture of the QCD vacuum. In particular, it was found in [11] that the mean instanton separation $R \approx 1.1 \text{fm}$ and the typical instanton radius $\rho \approx 0.35 \text{fm}$, about 10% off the values suggested by one of us a decade ago [12]. They also demonstrated explicitly how hadronic correlators 'survive cooling' and gave quite convincing arguments showing that confinement effects play only a relatively minor role.

In spite of such progress in phenomenology and lattice studies, a consistent quantitative theory of instanton-induced phenomena is still missing. The model mentioned above, RILM, assumes random instanton positions and orientations. It is clearly the simplest guess, the first step which ignores all effects related to instanton interactions. It seems to be a good approximation for multiple phenomena, but there are also important exceptions. In particular, finite temperature phenomena related to chiral symmetry restoration transition cannot be understood without the introduction of strong correlations between instantons and anti-instantons [13]. Furthermore, in the phase above $T_c$ these correlations are so strong, that they lead to breaking of the liquid into a set of weakly interacting $\bar{H}$ 'molecules'.

In this paper we discuss some global manifestations of the quark-induced interac-
tion between instantons in the $T = 0$ case. It is known that (in the chiral limit) they should screen large-scale fluctuations of the topological charge. As it is a very spectacular manifestation of dynamical correlations, it is natural to start our new series of studies of instanton-induced phenomena by reporting these results first. A detailed report on properties of the correlated instanton vacuum, including correlation functions and wave functions in particular channels, will be published elsewhere [14].

Before we proceed, let us remind why fluctuations of the topological charge are of interest. It is well known that strong interactions conserve CP to a high accuracy. Two ways to understand this 'fine tuning' were suggested. First, the $\theta$—parameter may set itself to zero due to the axion mechanism [15]. A new suggestions by Schierholtz [16] is that $\theta = 0$ may happen to be a phase transition point. In any case, there are all kind of open questions related to QCD at nonzero values of $\theta$, say whether it is a confining theory [16].

The second possibility is that the value of $\theta$ may be irrelevant because the total topological charge of the vacuum is screened completely. This happens if at least one quark flavor is massless, but this does not seem to be the case in the real world. Recently, a new proposal was put forward by Samuel [17] who argued that the interaction between instantons may screen the topological charge for non-zero quark masses, below some critical mass value.

Another important aspect is the famous U(1) problem [18, 19], related to properties of the $\eta'$ meson. Phenomenologically, its detailed properties are very important, for example for understanding of the so called 'proton spin crisis'. Theoretically, a recent discussion in connection with the Samuel mechanism can be found e.g. in [20, 21] in which the exchange of an $\eta'$ was interpreted as a mediator of the Debye-type screening. Generally speaking, the 'screening' phenomenon puts significant constraints on the parameters of this meson. Finite temperature effects in relation to the interpretation of the $\eta'$ particle as an inverse screening were discussed in [22].

A famous approach to the U(1) problem is based on the Witten-Veneziano formula [23, 24] relating the parameters of the $\eta'$ to the topological susceptibility $\chi$. Although it clearly explains qualitative features of the phenomenon, we cannot be satisfied by it. It is very difficult to make such type of relation quantitative because the two sides of the
equation 'live in two different worlds' \cite{20}. The parameters of the $\eta'$ meson are obtained from experiment and refer to the real world, while $\chi$ is calculated either in the large $N_c$ limit, or in quenched QCD \cite{25}, or in other non-screened theories. How one matches the unit of energy on both sides is therefore a matter of some convention.

No convincing lattice measurements of the $\eta'$ properties in QCD with dynamical fermions exist so far\textsuperscript{1}. In this paper we propose a method that does not require the inversion of the Dirac operator and might therefore be useful for lattice simulations.

The results for the $\eta'$ correlator in RILM \cite{4,5,6} are also unsatisfactory: the corresponding channel has shown to produce too strong $\bar{q}q$ repulsion. Besides that, the random ensemble has obviously no screening, so one cannot get any constraints related to it. Therefore, in this paper we study an ensemble of 'interacting instantons', and test whether and how the corresponding relations hold. An alternative approach to gluonic correlation functions, both in random and correlated instanton vacua, is developed in \cite{28}.

We suggest that the best way to clarify the issue is to study the dependence of topological susceptibility $\chi(V)$ defined in the sub-volume $V$. Its dependence on $V$, as well as on the quark masses $m_f$, are the main objective of our work. The screening of the topological charge implies that, for large $V$, $\chi(V)$ is proportional to the area of $V$ instead of $\chi(V) \sim V$, (see also \cite{26} where this phenomenon was discussed for the Schwinger model). However, for small volumes one always has that $\chi(V) \sim V$. The cross-over point between these two regimes defines a screening length, identified as the inverse $\eta'$ mass.

In section 2 we define the instanton liquid model and discuss the parameters used in our calculations. In section 3 the Debije cloud of a topological charge is studied and in section 4 the volume dependence of the topological susceptibility is evaluated. These results are analyzed in the context of correlators that follow from effective field theory (see appendix A). In section 5 we discuss the scalar gluonic correlation function which is related to the fluctuations of the total number of instantons in a given volume. Concluding remarks are made in section 6.

\textsuperscript{1}The best one so far is \cite{27}, where the $\eta'$ mass was calculated in quenched lattice gauge theory using a rather indirect method.
The model

The basis of this work is the ‘interacting instanton approximation’ (IIA), formulated as a particular statistical model amenable for numerical simulations [29, 30, 31] or analytical studies [32, 33]). The partition function for \( N/2 \) instantons and \( N/2 \) anti-instantons is generally given by

\[
Z = \int d\Omega_I d\rho_I \mu(\rho_I) \prod_{I=1}^N \det(T + im_f) \exp\left[-\beta(\rho\Lambda) \sum_{I<J} S_{IJ}^{\text{int}}\right],
\]

(2.1)

where \( \Omega_I, z_I \) and \( \rho_I \), denote the orientation, position and the size of pseudoparticle \( I \), respectively. The size distribution \( \mu(\rho) \) contains a factor \( \sim \rho^{b-5} \) (with the standard beta-function parameter \( b = \frac{11}{3}N_c - \frac{2}{3}N_f \)) due to Jacobian of the transformation to collective coordinates and the leading quantum corrections (\( \beta(\rho\Lambda) = -b \log(\rho\Lambda) \)). The QCD parameter \( \Lambda \) will be determined phenomenologically.

The main dynamical effects we are going to study are due to the determinant of the Dirac operator. In the subspace of the zero modes it can be expressed in terms of the overlap matrix elements \( T \), which for the ‘streamline’ gauge fields [34] are given by [35]

\[
T_{AI}(\rho_I\rho_A)^{1/2} = (\rho_I\rho_A)^{1/2} \int d^4x \bar{\psi}_0^A(x)i\gamma_5 \psi_0^I(x) = \frac{1}{2} Tr \left( \gamma_\mu R^A_{\mu} U_I^{-1} U_A \right) F(\lambda),
\]

(2.2)

where the scalar function \( F(\lambda) \) is defined by

\[
F(\lambda) = 6 \int_0^\infty \frac{dr r^{3/2}}{(r + 1/\lambda)^{3/2}(r + \lambda)^{5/2}}.
\]

(2.3)

It depends on the conformally invariant combination \( \lambda \)

\[
\lambda = \frac{1}{2} \left( \frac{\tilde{R}^2 + \rho_I / \rho_A}{\rho_A / \rho_I} \right) + \frac{1}{2} \left( \frac{(\tilde{R}^2 + \rho_I / \rho_A)^2 - 4}{\rho_A / \rho_I} - 4 \right)^{1/2},
\]

(2.4)

where \( \tilde{R} = R / \sqrt{\rho_I \rho_A} \). Asymptotically, for large \( R/\rho \), the \( T_{AI} \sim 4\rho^3/R^3 \) (the geometric average of \( \rho_I \) and \( \rho_A \) id denoted by \( \rho \)).

Considering the interaction due to gauge fields, let us first mention that we deviate from previous works\(^2\) by using the interaction derived in [34] from the so called ‘streamline equation’ [36]. They correspond to the true bottom of the valley for the \( \bar{I}I \)-configurations.

\(^2\)They used variational trial functions for the gauge fields known as the ‘sum’ or ‘ratio’ ansatz.
This interaction differs from the previously used ones in one important aspect: for one relative orientation the repulsive ‘core’ at small distances is gone. Our numerical simulations have confirmed earlier suspicions that it leads to an ‘overcorrelated liquid’ of close $\bar{I}I$ pairs. It is still possible, that one may get a phenomenologically acceptable ensemble by a significant increase in the density of instantons. However, to spend a major portion of computer time simulating pairs that are not even semiclassical fluctuations is not practically possible.

Thus, it seems that the original hopes to stabilize the ensemble at the purely classical level [32] are not fulfilled. Presumably quantum effects (especially subtraction of perturbative contributions, relevant for close instanton-anti-instanton pairs with a strongly attractive interaction) will generate the effective repulsion, and two recent developments should be mentioned in this context. First, Diakonov and Petrov calculated the instanton interaction from the semiclassical quark scattering amplitude [37] and found a short range repulsion. However, at the moment it is not yet clear to what extent this interaction is of relevance to the present problem. Second, some quantum corrections, discussed in [38] using the scale anomaly relation, also lead to some effective repulsion.

Lacking a detailed understanding of these effects, we have introduced a phenomenological repulsive core [3] to the streamline action $S^{SL}(\lambda)$

$$S_{IA}^{int} = S^{SL}(\lambda) + \frac{A}{2\lambda^4} \text{Tr} 12U_I^{-1}U_A12U_A^{-1}U_I,$$  

$$S_{II'}^{int} = \frac{A}{2\lambda^4} \text{Tr} 12U_I^{-1}U_I'12U_{I'}^{-1}U_I,$$  

for pseudoparticles of the opposite and identical kind, respectively. (In the latter case the classical interaction is absent and only the hard core is included.) The strength of the core is denoted by a free parameter $A$, and the color traces are needed to reduce the magnitude of the interaction if two pseudoparticles belong to different SU(2) subgroups of $SU(N_c)$.

In principle, $A$ determines the total instanton density in terms of $\Lambda_{QCD}^4$. Unfortunately, it is not known with sufficient accuracy, and therefore it is logical to do the same thing as on the lattice, namely tune those two parameters to some measured masses, and then

---

3Let us point out an analogy to the famous problem of nuclear matter saturation: although there is no doubt for the existence of a repulsive core for NN forces and its decisive role in the problem, its properties and physical nature is debated even today, after decades of investigations!
consider others as predictions. This strategy will be used in a subsequent work on hadron spectroscopy in the IIA.

However, in this paper, related to only a limited number of issues, we adopt a simpler normalization prescription. For all masses, number of colors or flavors we (i) fix the total density of the instantons at \( n = 1\,fm^4 \), roughly corresponding to the standard gluon condensate value and to lattice measurements; (ii) the repulsive core strength is fixed to be \( A = 128 \), for which we obtain a \textit{quark condensate} that is close to the empirical value. (Note that in this region the dependence on \( A \) is relatively weak.)

We simulate the partition function with a Metropolis algorithm for an ensemble of \( N/2 = 32 \) instantons and an equal number of anti-instantons in a box of size \((2.38\,fm)^3 \times 4.76\,fm\). We average over typically 1,000 statistically independent configurations.

### 3 Screening of the topological charge

Let us start with the evaluation of the topological charge

\[
Q(l_4) = \int_{H(l_4)} d^4x \frac{g^2}{32\pi^2} F\tilde{F}(x),
\]

in a subvolume ('slice' of the box) \( H(l_4) \equiv L^3 \times l_4 \). It is not an easy task on a lattice, but for our instanton ensemble this simplifies to just counting instantons and anti-instantons with centers in the subvolume.

Our aim is to study the details of the screening phenomenon such as the \textit{size} and \textit{shape} of the corresponding 'Debye cloud'. Let us take the center of one of the anti-instantons as the origin of the coordinate system and measure the charge distribution in the rest of the system. In Fig. 1 we show results of such studies for \( N_c = 3 \) and \( N_f = 2 \) (both u,d quarks with equal masses, given in the label of the figures). Since the total charge in the box is set to zero, the 'compensating charge' contained in the slice \( H(l_4) \) for large enough \( L_4 \) should approach 1 (the anti-instanton in the center is not counted).

Our data (points) do show a strong screening phenomenon, namely that most the compensating charge is contained in rather small slice of the box, with a width of only
about 1/3 fm. That means that the correlations between instantons and anti-instantons, responsible for screening, are actually very short range ones. The relevant hadronic excitation, the pseudo-scalar flavor singlet channel, should therefore be relatively heavy. Thus, our ensemble solves the U(1) problem at least qualitatively.

One more qualitative phenomenon to mention here is the observed charge oscillations around the central charge. Those are well seen for $m = 0$, and fade away for larger masses. The oscillations are clearly non-statistical, and their appearance suggests that in the 'instanton liquid' there exist correlated clusters of various sizes. Let us recall in this connection, that in many ordinary liquids one finds local order characteristic to a crystalline phase, and that clusters can be as big as containing hundreds of atoms. This interesting topic clearly deserves further studies.

Doing a more quantitative analysis, we have fitted these data by the function

$$Q(l_4) = \alpha^2(1 - \exp(-ml_4)) + (1 - \alpha^2)\frac{l_4}{L}$$  \hspace{1cm} (3.2)

The fraction $\alpha$ is the magnitude of the 'compensating charge', if $\alpha = 1$ the charge is screened completely. The second term corresponds to the remaining charge which is assumed to be distributed homogeneously over the box. The first term is obtained by integrating the correlation function (A.13) for fixed $x_4 - y_4 = l_4$. In the effective low energy field theory (discussed in appendix A) the mass $m$ is identified as the $\eta'$ mass.

The obtained values for $\alpha$ are 1.0, 0.99, 0.96 and 0.80 for the 4 masses used ($m = 0.0, 0.1, 0.2$ and 0.4 in units of $fm^{-1}$), with statistical errors about 0.05. Thus, the non-screened charge $(1 - \alpha^2) \sim m^\delta$ with the power $\delta = 1$ to 2. This conclusion should be compared to the conventional wisdom, according to which it should be proportional to the lightest quark mass. We do not know whether there is a discrepancy, or that it is due to finite size effects (the $1/L$ term in (3.2)). In the scenario proposed by Samuel, the effect should vanish at a non-zero critical mass $(1 - \alpha^2) \sim (m - m_c)^\delta$. Our results lead to an upper limit of about $m_c < 20 MeV$.

The value of the second parameter, $m_{\eta'}$, equals 673, 623, 555 and 518 MeV, in these 4 cases, respectively\footnote{We remind the reader that the 'MeV' makes sense in those un-physical theories only after we have defined them, rather arbitrarily, by keeping the density of instantons fixed at some value. Comparison to lattice simulations is possible, but one has to keep the same convention. The physical situation will be discussed below.}. The result is that singlet mass decreases with the current quark
mass and suggests that the screening length becomes larger if one is increasing all quark masses.

4 Fluctuations of the topological charge in a subvolume

In this section we switch to more conventional observables, which have been discussed in both theoretical and lattice literature. They are closely related to what was done above, but at the same time they do not demand the charge to be localized.

Although the average value of the topological charge in some volume is, of course, zero, one may study its fluctuations $\langle Q^2 \rangle$. More specifically, we study the dependence on the finite volume $V_4$, its surface $A_3$, etc.,

$$\langle Q^2 \rangle_{V_4} = C_V(m) V_4 + C_A(m) A_3.$$  \hfill (4.1)

(The subscripts refer to the dimensions of the manifolds).

We have already mentioned, that the attention in literature has been focused on the large volume limit of that quantity, the topological susceptibility

$$\chi = \lim_{V_4 \to \infty} \frac{\langle Q^2 \rangle_{V_4}}{V_4}.$$  \hfill (4.2)

The dependence of $\chi$ on the quark masses $m$ is the same as for unscreened charge $1 - \alpha^2$ discussed above: the standard scenario with the 'screening of the topological charge' implies that $\chi \sim m$ at small $m$, while in Samuel’s scenario $\chi = 0$ for all quark masses below some critical value $m < m_c$.

Our idea is to study not only the limiting value of the topological susceptibility but its dependence on the subvolume. The particular behavior to be observed is very informative, and can be used to extract additional information about vacuum properties (and hadronic spectroscopy). Specifically, as we try to separate volume from surface effects, we take a segment of the hypertorus of variable length $l_4$ along the 4-axis, i.e. the slice $H(l_4)$ discussed in previous section. Its total volume $L^3 l_4$ is proportional to $l_4$, while its surface area $L^3$ is independent of it. Because our box size in the 4-direction is $L_4 = 2L$, the effective range of $l_4$ is $0 < l_4 < L$. 

9
Furthermore, as we have seen in appendix A, the topological correlation function
\[ \Pi_P(x - y) \] (see (A.13)) can be connected with parameters of the SU(3)-scalar pseudoscalar mesons, the famous \( \eta' \)–particle and the corresponding excited states.

The fluctuations of the charge \( Q(l_4) \) in the box \( H(l_4) \) are obtained by integrating the correlation function (A.13):
\[ K_P(l_4) \equiv \langle (Q(l_4))^2 \rangle = L^3 \int_{L^3} d^3 x \int_{-l_4}^{l_4} dt (l_4 - |t|) \Pi_P((\vec{x}^2 + t^2)^{\frac{1}{2}}). \] (4.3)

This integral vanishes for \( l_4 \to \infty \) if any quark becomes massless\(^5\) (see eq. (A.15) in appendix A). For finite \( l_4 \) this integral can be done as well; for sufficiently large \( L \gg 1/m \) the range of the spatial integration can be extended to infinity with high accuracy \( O(\exp(-L m_{\eta'})) \) and the result is
\[ \langle (Q(l_4))^2 \rangle = L^3 n \left[ l_4 + \cos^2 \phi \frac{m_{\eta'}^2}{m_\eta} \left( \frac{1 - \exp(-m_{\eta'} l_4)}{m_{\eta'}} - l_4 \right) + \sin^2 \phi \frac{m_4^2}{m_\eta} \left( \frac{1 - \exp(-m_{\eta} l_4)}{m_{\eta}} - l_4 \right) \right]. \] (4.4)

For \( l_4 \to 0 \) we find
\[ \langle (Q(l_4))^2 \rangle = n L^3 l_4. \] (4.5)

One can easily convince oneself that this result is independent of the specific shape of the subvolume, and in general we have
\[ \lim_{V \to 0} \frac{\langle (Q(V))^2 \rangle}{V} = n. \] (4.6)

Together with eq. (A.14), this results in the following formula for the \( \eta' \) mass
\[ m_{\eta'}^2 + m_{\eta'}^2 - m_R^2 = \frac{2N_f}{f^2} \lim_{V \to 0} \frac{\langle (Q(V))^2 \rangle}{V}, \] (4.7)

which is our analog of Witten-Veneziano formula, with the topological susceptibility replaced by local fluctuations of the topological charge. It should hold for volumes in the window between that of a single instanton \( O(\rho^4) \) and the inverse of their density \( O(1/n) = O(R^4) \).

In terms of the flavor singlet spectral function, the correlation function (L.4) implies that neither the contribution of the \( \iota \) nor the contribution of the continuum have been

\(^5\)A similar cancellation takes place in many cases, e.g. in (2-d) Schwinger model (see [26] for details).
taken into account. We only calculate the non-perturbative contribution to the correlation function \( \Pi_P^{NP} = \Pi_P - \Pi_P^{pert} \) which implies that the contribution of the continuum and the resonances appear with opposite signs in \( \Pi_P^{NP} \). In particular we will find a cancellation between the \( \iota \) and the continuum. In the fits to be discussed below we included the contribution of the continuum, and in all cases we found that the best fit was obtained for zero coupling of the continuum. From now on we do not include it in our discussion.

Our results for the fluctuations of the topological charge, \( K_P(l_4) \), in a slice with length \( l_4 \) are shown in Figs. 2, 3 and 4. The first qualitative point we would like to make is that the data points clearly show the expected transition from a linear dependence on \( l_4 \) (for small box size) to a constant for larger boxes (in case the quark mass is zero). These data point deviate drastically from the full line corresponding to randomly positioned instantons\( ^6 \), the behaviour that holds for the RILM used in \([4, 5, 6]\). Thus, the topological charge is in fact screened and its fluctuations become a surface rather then a volume phenomenon, as soon as the quark-induced interactions are included in the statistical sum.

In the upper figure of Fig. 2 we compare the cases with one and two massless quarks, for \( N_c = 2 \). For massless quarks the correlation function \([14]\) reduces to

\[
\langle Q(l_4)^2 \rangle_{\text{chiral}} = \frac{1 - \exp(-m_{\eta} l_4)}{m_{\eta}'}.
\]

The dashed curves show a fit of this function to the data points. For \( N_f = 1 \) and \( N_f = 2 \) we find \( m_{\eta}' = 535 \text{MeV} \) and \( m_{\eta}' = 756 \text{MeV} \), respectively. The ratio of the masses is 1.41 which is right on top of the theoretical expectation that \( m_{\eta}' \sim \sqrt{N_f} \) (see \([A.14]\)). If we study the susceptibility \( \langle Q(l_4)^2 \rangle \) as a function of the quark mass, which effectively reduces the number of flavors, we therefore expect on the one hand that the \( \eta' \) mass decreases, whereas, on the other hand, it increases because of the explicit contribution of the quark masses.

The quark mass dependence of the topological correlator is studied in Fig. 3. In this case the number of colors is 3 and we consider two flavors with equal mass (same instanton configurations as in Fig. 1). For the quark mass we refer to the label of the figure.

\( ^6 \) The functional form of this curve, which follows immediately from the binomial distribution of the instantons, is given by \( N(l_4/L_4)(1 - (l_4/L_4)) \).
In the case of equal quark masses, the fitting formula (that follows from eq. A.13) is
\[
\langle Q(l_4)^2 \rangle = n L^3 \left( \alpha^2 l_4 (1 - \frac{l_4}{2L}) + (1 - \alpha^2) \frac{1 - \exp(-m_{\eta'} l_4)}{m_{\eta'}} \right).
\] (4.9)

The value of \( \alpha \) obtained from a least square fit is 0.0, 0.0, 0.0, 0.19 and \( m_{\eta'} \) equals 580, 520, 430 and 340 MeV for quark masses of 0.0, 20.0, 40.0 and 80.0 MeV, in this order. As we already observed in previous section, our results set a limit on the existence of a critical mass below which we have complete screening. Again with the disclaimer that the individual parameters are not well determined by the fit. Only the height of the curves is well-determined. Our values for the \( \eta' \) mass are somewhat less than in previous section, but show the same trend that it decreases for not too large quark masses.

Finally, in Fig. 4, we show results for realistic quark masses, \( m_u = m_d = 10 \text{MeV} \) and \( m_s = 150 \text{MeV} \). The dashed line corresponds to effective theory with realistic meson masses and \( \eta-\eta' \)-mixing angle. The full line is a fit of eq. (4.4) to the data. Both the pion and the kaon mass are found to be zero, whereas \( m_{\eta'} = 605 \text{MeV} \). Also in this case the individual parameters are not well determined by the fit. In particular, the fitted curve is very insensitive to the value of the strange quark mass. In fact, the best fit misses the strange quark contribution to the \( m_{\eta'} \). Note that in naive chiral perturbation theory this meson should possess a strangeness-related mass \( m_{\eta'}^{\text{strange}} = m_{\eta}/\sqrt{2} = 388 \text{MeV} \). The sum of these two numbers are right in the correct region.

5 Compressibility of the instanton liquid

Let us now proceed to studies of a related gluonic correlation function
\[
\Pi_S(x - y) = \langle \frac{g^2}{32\pi^2} FF(x) \frac{g^2}{32\pi^2} FF(y) \rangle,
\] (5.1)
containing the action rather than the topological charge, and therefore counting instantons and anti-instantons equally. The total topological charge in a subvolume \( V \) is given by
\[
N(V) = \int_V d^4x \frac{g^2}{32\pi^2} FF(x),
\] (5.2)
\footnote{Of course, for any finite volume simulation the value of \( m_f \) cannot be taken arbitrary small: the minimum possible value of \( m \) is the point where the \( m \)–derivative of the condensate vanishes. For feasible volumes we work with \( m_f = 0.05 \approx 10 \text{MeV} \), being small compared to hadronic masses but still considerably larger than the light quark masses in the real world.}
which satisfies that \(<N(V)> = nV\). For pointlike pseudoparticles we have
\[
\frac{g^2}{32\pi^2} FF(x) = \sum_{I=1}^{N} \delta^4(x - X_I).
\] (5.3)

For small \(|x - y|\) only terms involving the same instanton contribute and we find that\(^8\)

\[
\Pi_S(x - y) = n\delta^4(x - y) \quad \text{for} \quad |x - y| \to 0.
\] (5.4)

In reality the instantons are not pointlike, and show a repulsive interaction. This leads to the low-energy theorem \([1, 32, 44]\)
\[
\langle [N(V)]^2 \rangle - \langle N(V) \rangle^2 = \frac{4}{b} \langle N(V) \rangle,
\] (5.5)

for \(V \to \infty\). The compressibility of the instanton liquid is thus equal to \(4/b\). As can be seen from (5.4), for small volumes the factor \(4/b\) is absent. How can we understand this in terms of the physical states contributing to the correlation function? The lowest lying intermediate state is a 'scalar glueball', which we will generically call \(\sigma\) (not to be mixed with the \(\sigma\) of sigma-model, at 600 MeV). Using a somewhat different convention than in the pseudoscalar channel the relevant matrix element is

\[
\langle 0 | \frac{g^2}{32\pi^2} FF | \sigma \rangle = \lambda_\sigma.
\] (5.6)

Including the contact term and the contribution of the continuum with coupling constant \(\lambda_c\), this results in the correlator

\[
\Pi_S(x - y) = n\delta^4(x - y) + \lambda_\sigma^2 D(m_\sigma, |x - y|) + \lambda_c^2 \int_{s_0}^{\infty} ds D(\sqrt{s}, |x - y|) s^2.
\] (5.7)

This result contains both perturbative and nonperturbative contributions. However, the correlation function that is obtained from the instanton liquid calculation only receives contributions from the latter sector. Therefore, we should compare out results to \(\Pi_S^{NP} \equiv \Pi_S - \Pi_S^{pert}\). The spectral representation of the perturbative contribution is given by

\[
\Pi_S^{pert} = \lambda_c^2 \int_{0}^{\infty} ds D(\sqrt{s}, |x - y|) s^2.
\] (5.8)
In the same way as for the topological correlator we define the correlator, \( K_S(l_4) \), as the \textit{variance} of the total field strength inside the box \( H(l_4) \). Numerically, this correlator can be evaluated again by simply counting the number of instantons inside the box. It is related to \( \Pi_{S}^{\text{NP}} \) by

\[
K_S(l_4) = L^3 \int_{L^3} d^3 x \int_{-l_4}^{l_4} dt (l_4 - |t|) \Pi_{S}^{\text{NP}}((\bar{x}^2 + t^2)^{\frac{1}{2}}).
\]

(5.9)

Using the the correlators (5.7, 5.8) we find

\[
K_S(l_4) = nL^3 l_4 + \lambda_{\sigma}^2 L^3 (l_4 - \frac{1 - \exp(-m_{\sigma} l_4)}{m_{\sigma}}) - \lambda_{c}^2 L^3 \int_{0}^{\infty} (l_4 - \frac{1 - \exp(-l_4 \sqrt{s})}{\sqrt{s}}) s^2 ds.
\]

(5.10)

For large volumes the low-energy theorem (5.5) should be obeyed. This leads to the relation

\[
n + \lambda_{\sigma}^2 - \lambda_{c}^2 = \frac{4}{b} n,
\]

(5.11)

which shows that in the scalar case (in contrast to pseudoscalar one treated above) it is essential to include the contribution of the continuum. (Recall also that in the pseudoscalar case the sign of contribution from the \( \eta' \) resonance is negative due to the anti-hermiticity of \( F \bar{F} \).)

In the lower figure of Figs. 2 and 4 and Fig. 5, we show results for the scalar correlators. The full lines in all figures correspond to a random positioning of the instantons. For infinite volume we would get a straight line, but finite size corrections turn it into a parabola. The numerical results are represented by dots, and the dashed line is a fit using the function

\[
f(l_4) = \frac{N}{2L} \left( \frac{4}{b} l_4 (1 - \frac{l_4}{2L}) - \lambda_{\sigma}^2 1 - \frac{\exp(-m_{\sigma} l_4)}{m_{\sigma}} + \frac{4}{\sqrt{s_0}} (1 + \lambda^2 - \frac{4}{b}) F(l_4 \sqrt{s_0}) \right),
\]

(5.12)

where the 'missing continuum function' \( F \) follows from the integral in (5.10)

\[
F(x) = \frac{1}{3} + \frac{2}{x^3} - \left( \frac{1}{x} + \frac{2}{x^2} + \frac{2}{x^3} \right) \exp(-x)).
\]

(5.13)

This fitting function both reproduces the short distance behavior (5.4) and the low-energy theorem (5.5).

Results for \( N_c = 2 \) and \( N_f = 1 \) or \( N_f = 2 \) are shown in Fig. 4. Two fits with comparable \( \chi^2 \) but very different parameters are found. First, we a fit with \( \lambda = 0 \) and
$\sqrt{s_0} = 1110$ MeV for $N_f = 1$ and 715 MeV for $N_f = 2$, respectively. In this case $m_\sigma$ is indeterminate. A second minimum is found for $\lambda = 1.22$ and $m_\sigma = \sqrt{s_0} = 2.4$ GeV for $N_f = 1$ and $\lambda = 1.32$ and $m_\sigma = \sqrt{s_0} = 1.9$ GeV. In both cases, the bulk of the $l_4$ behavior is determined by the low-energy theorem, and the resonance and continuum only contribute significantly for small volumes.

In Fig. 5 we study the current quark mass dependence for $N_c = 3$ and two flavors of equal mass. Again we find two different fits. First, for current quark masses equal to 0, 20, 40 and 80 MeV we find a fit with $\lambda = 0.0$ and $\sqrt{s_0}$ equal to 1160, 1295, 1245 and 1525 MeV, respectively, and, second, we find $\lambda = 1.56, 1.60, 1.44$ and 1.72 and $m_\sigma = \sqrt{s_0} = 2.6, 2.9, 2.6$ and 3.7 GeV, in the same order. In both cases, the bulk of the correlation function is determined by the low-energy theorem (5.5).

Finally, in the lower figure of Fig. 3, we show $K_S$ for realistic values of the quark masses (see caption). As a best fit with $\lambda = 0$ we find that $\sqrt{s_0} = 1320$ MeV. For the fit with $m_\sigma = \sqrt{s_0}$ we find a mass of 2.97 GeV and a coupling constant of $\lambda = 1.53$. These results are consistent with the factor $4/b$ in the low-energy theorem.

We want to emphasize that the value $\lambda = 0$ and the equality $m_\sigma = \sqrt{s_0}$ are a result of the fit. The fits quoted here are not the only fits; there are other minima of $\chi^2$ which we dismissed as unphysical. For example, in the last case is also fitted by $\sqrt{s_0} = \frac{4}{3}m_\sigma = 200$ MeV and $\lambda = 4.5$. For this ratio of the masses the asymptotics of the fitting function becomes independent of $\lambda$. Therefore the conclusion that the bulk of the results are described by the low-energy theorem remains unaffected.

6 Conclusions

We have presented a detailed study of the volume dependence of the fluctuations of the topological charge in an Interaction Instanton Approximation to the QCD vacuum. As was expected, we found that these fluctuations are screened for a sufficiently large box and sufficiently small quark masses due to the fermion-induced interaction between instantons. The phenomenon disappeared gradually as the quark mass increases from zero. An upper limit for the Samuel’s critical mass value is set to about 20 MeV. Furthermore, the results
for a correlated instanton liquid have shown that correlations are essential for reproducing the $m'_\eta$ and its dependence on the number of colors and flavors in the theory.

As a by-product, we have obtained a formula similar to the Witten-Veneziano formula, but the topological susceptibility that enters into it is not the large volume limit but rather the small volume limit in the presence of dynamical fermions.

We also present results for the fluctuations of total number of instantons in the finite box. The results clearly indicate that the instanton liquid is not an ideal gas, but a liquid with an important repulsive interaction. The results agree very well with the NSVZ low-energy theorem, and provide constraints for the parameters of the physical particles in the scalar channel.

Finally, let us emphasize that the method to evaluate the $\eta'$ parameters proposed in this work can be applied to lattice QCD calculations with dynamical fermions as well. Straightforward evaluation of the quark propagators can be substituted by measurements of the topological charge in a finite box, which may be much easier to do.

Acknowledgments

This work was supported in part by the US department of energy under Grant DE-FG02-88-ER40388. We acknowledge the NERSC at Lawrence Livermore where most of the computations presented in this paper were performed. Th. Schäfer and I. Zahed are acknowledged for useful discussions.

Appendix A: Topological correlators in effective field theory

The topological charge density is defined by

$$Q(x) = \frac{g^2}{32\pi^2} F \bar{F}(x), \quad (A.1)$$

where $F$ is the field strength tensor. The topological charge $Q(V)$ in 4-volume $V$ is obtained by integration of $Q(x)$ over $V$. The fluctuations of the topological charge in a
given box are determined by the topological correlation function defined by
\[ \Pi_P(x - y) = \langle \frac{g^2}{32\pi^2} F^a(x) \frac{g^2}{32\pi^2} F^a(x) \rangle. \] (A.2)

In this appendix we will derive this correlator from the effective low-energy chiral Lagrangian [39] and its interaction with the topological charge \( Q \). This derivation is based on work in references [19, 20, 21]. The main additional ingredient is that we include the \( \eta - \eta' \) mixing in our derivation.

The topological charge density couples to the pseudoscalar singlet meson channel, and, for a diagonal mass matrix with \( m_u = m_d \), only the \( \eta - \eta' \) mixing part of the effective pseudoscalar Lagrangian is of relevance. This part, which involves only the diagonal \( SU(3) \)-flavor fields \( \phi_0 \) and \( \phi_8 \), is given by [24, 39, 40, 33, 41]
\[ L_{\text{eff}} = -i \int d^4x \sqrt{\frac{2N_f}{f}} \phi_0 Q + L(\phi_0, \phi_8), \] (A.3)
with
\[ L(\phi_0, \phi_8) = \frac{1}{2} \left( \begin{array}{c} \phi_0 \\ \phi_8 \end{array} \right) \left( \nabla^2 + M^2 \right) \left( \begin{array}{c} \phi_0 \\ \phi_8 \end{array} \right), \] (A.4)
and the square of the mass matrix [24]
\[ M^2 = \begin{pmatrix} \frac{\sqrt{2}}{3}m_K^2 + \frac{1}{3}m_\pi^2 & \frac{2\sqrt{2}}{3}(m_\pi^2 - m_K^2) \\ \frac{2\sqrt{2}}{3}(m_\pi^2 - m_K^2) & \frac{4}{3}m_K^2 - \frac{1}{3}m_\pi^2 \end{pmatrix}. \] (A.5)

The normalization of the fields and the coupling constant \( f \) will be discussed below.

In the dilute gas approximation the instanton partition function is given by [42, 19]
\[ Z = \sum_{N_+,N_-} \frac{\kappa^{N_+ + N_-}}{N_+!N_-!} \prod_{i=1}^N d^4 z_i \exp(- \int d^4x L_{\text{eff}}). \] (A.6)

The constant \( \kappa \) was calculated to one loop order in [3]. Treating the instantons as pointlike objects, the topological charge density is given by \( Q(x) = \sum Q_i \delta(x - z_i) \). This allows us to perform the sum over \( N_+ \) and \( N_- \) in the partition function. Our final effective Lagrangian is obtained by expanding the resulting cosine-function to second order (weak field approximation):
\[ L_{\text{eff}} = -2V\kappa + \frac{2N_f}{f} \phi_0^2 + L(\phi_0, \phi_8). \] (A.7)

\(^{9}\text{In fact, there is another state with the quantum numbers of the } \eta', \eta(1430) \text{ and formerly called } \iota, \text{ which gives a comparable contribution to this correlation function (see discussion in [3]). We do not include it here, because it is hardly possible to extract any information about this state from the data sample discussed in this paper.}\)
The constant $\kappa$ can be traded for the average pseudoparticle density by differentiating both (A.6) and (A.7) with respect to $\kappa$. We find

$$2\kappa = \langle \frac{N}{V} \rangle \equiv n.$$  \hspace{1cm} (A.8)

The topological correlator (A.2) can be obtained by integrating out the meson fields. However, it is somewhat simpler to write the correlator in terms of functional derivatives with respect to $\phi_0$ of the first term in the Lagrangian (A.3) and performing the differentiation after the sum over the instantons, i.e. on the second term in (A.7). The correlator can be expressed as

$$\langle Q(x)Q(y) \rangle = n\delta^4(x-y) - n^2\frac{2N_f}{f^2} \langle \phi_0(x)\phi_0(y) \rangle.$$  \hspace{1cm} (A.9)

The latter expectation value is most conveniently obtained by diagonalizing the mass matrix $\mathcal{M}$ (including the topological contribution) with eigenvalues identified as $m_{\eta'}$ and $m_{\eta}$ and eigenvectors expressed in the $\eta' - \eta$ mixing angle according to

$$|\eta' \rangle = \cos \phi |\phi_0 \rangle + \sin \phi |\phi_8 \rangle,$$

$$|\eta \rangle = \cos \phi |\phi_8 \rangle - \sin \phi |\phi_0 \rangle.$$  \hspace{1cm} (A.10-11)

For the singlet correlation function we obtain

$$\langle \phi_0(x)\phi_0(y) \rangle = \cos^2(\phi)D(m_{\eta'}|x-y|) + \sin^2(\phi)D(m_{\eta}|x-y|)$$  \hspace{1cm} (A.12)

resulting in the topological correlator

$$\langle Q(x)Q(y) \rangle = \frac{f^2}{2N_f}m_{\top}^2 \left[ \delta^4(x-y) - m_{\top}^2 (\cos^2(\phi)D(m_{\eta'}|x-y|) + \sin^2(\phi)D(m_{\eta}|x-y|)) \right],$$  \hspace{1cm} (A.13)

where the scalar propagator is given by $D(mx) = mK_1(mx)/(4\pi^2x)$. For convenience we have introduced the topological mass

$$m_{\top}^2 \equiv \frac{2N_f n}{f^2} = m_{\eta'}^2 + m_{\eta}^2 - 2m_K^2,$$  \hspace{1cm} (A.14)

where the latter identity follows from the invariance of the trace of the mass matrix under diagonalization. This correlation function can also be derived from the pseudoscalar...
singlet spectral function with the matrix element \( \langle 0|Q(x)|\eta' \rangle = m_{\eta'}^2 f_{\eta'}/\sqrt{2N_f} \). This defines the constant and the normalization of the fields in our effective Lagrangian.

It is interesting to calculate the topological susceptibility

\[
\chi \equiv \lim_{V \to \infty} \frac{\langle (\int d^4x Q(x))^2 \rangle}{V} = \frac{f^2}{2N_f} m_{\text{top}}^2 \left( 1 - \frac{\left( \frac{4}{3} m_K^2 - \frac{1}{3} m_{\pi}^2 \right) m_{\text{top}}^2}{\left( \frac{4}{3} m_K^2 - \frac{1}{3} m_{\pi}^2 \right) m_{\text{top}}^2 + 2 m_K^2 m_{\pi}^2 - m_{\pi}^4} \right) \tag{A.15}
\]

We observe the well-known fact that the topological charge is completely screened if one massless quark is present. Note that this formula has been derived for \( m_u = m_d \). Indeed, for zero light quark masses we have \( m_{\pi} = 0 \) and \( \chi = 0 \). If \( m_s = 0 \) we have that \( m_{\pi}^2 = 2 m_K^2 \) and also \( \chi = 0 \).

As has been particularly emphasized by Dowrick and McDoughal [20], we can look at the effective Lagrangian in a different way. Namely we integrate over the pseudoscalar singlet and are left with a residual instanton interaction. In the present case, with the \( \eta' - \eta \) taken into account, we have to integrate over both \( \phi_0 \) and \( \phi_8 \). This results in the effective lagrangian

\[
\mathcal{L} = \frac{1}{2} \frac{2N_f}{f^2} \sum_{ij} Q_i Q_j \left( \cos^2 \phi D(m_{\pi}|z_i - z_j|) + \sin^2 \phi D(m_K|z_i - z_j|) \right). \quad \tag{A.16}
\]

The range of the interaction between the pseudoparticles is of order of \( 1/m_{\pi} \). Ignoring the the \( \eta' - \eta \) mixing would have led to the improper conclusion [22] that interaction range of \( 1/m_K \). Although it is believed that a Yukawa interaction is not strong enough [13] to induce a plasma phase, the relatively long range interaction justifies the study of the scenario recently proposed by Samuel [17].
References

[1] V. Novikov, M. Shifman, A. Vainshtein and V. Zakharov, Nucl. Phys. B165 (1980) 67.

[2] A.A. Belavin, A.M. Polyakov, A.A. Schwartz and Yu.S. Tyupkin, Phys. Lett. 59B (1975) 85.

[3] G. ’t Hooft, Phys. Rev. Lett. 37 (1976) 8; Phys. Rev. D14 (1976) 3432.

[4] E.V. Shuryak and J.J.M. Verbaarschot, Nucl. Phys. B 410 (1993) 37.

[5] E.V. Shuryak and J.J.M. Verbaarschot, Nucl. Phys. B 410 (1993) 55.

[6] T. Schäfer, E.V. Shuryak and J.J.M. Verbaarschot, Nucl. Phys. B 412 (1994) 143.

[7] E. V. Shuryak, Rev. Mod. Phys. 65, 1 (1993)

[8] M.C. Chu, J.M. Grandy, S. Huang, and J.W. Negele, Phys. Rev. Lett. 70, 255 (1993)

[9] T. Schäfer, E. V. Shuryak, Hadronic Wavefunctions in the Instanton model, preprint, SUNY-NTG94-5, hep-ph/9401289.

[10] B. Berg, Phys. Lett. B114, 475 (1981); M. Teper, Nucl. Phys. B20 (Proc. Suppl.), 159 (1991).

[11] M. C. Chu, J. M. Grandy, S. Huang, J. W. Negele, preprint, MIT-CTP#2269, hep-lat/9312071

[12] E. V. Shuryak, Nucl. Phys. B203, 116, 140, 237 (1982)

[13] T. Schäfer, E.V. Shuryak and J.J.M. Verbaarschot, Nucl. Phys. B 412 (1994) 143.

[14] T. Schäfer, E.V. Shuryak and J.J.M. Verbaarschot, Mesons in the correlated instanton vacuum.

[15] R. Peccei and H. Quinn", Phys. Rev. Lett. 38 (1977) 1440

[16] G. Schierholtz, Towards a dynamical solution of the strong CP problem, DESY preprint DESY 94-031 (1994).

[17] S. Samuel, Mod. Phys. Lett. A7 (1992) 2007.

[18] S. Weinberg, Phys. Rev. D11 (1975) 3583.

[19] G. ’t Hooft, Phys. Rep. 142 (1986)357.

[20] N.J. Dowrick and N.A. Mcdougall, Phys. Lett. B285 (1992) 269; Nucl. Phys. B399 (1993) 426.

[21] H. Kikuchi and J. Wudka, Phys. Lett. B284 (1992) 111.
[22] I. Zahed, \textit{QCD instantons in vacuum and matter}, Stony Brook preprint SUNY-NTG-94-22.
[23] E. Witten, Nucl. Phys. \textbf{156} (1979) 269.
[24] G. Veneziano, Nucl. Phys. B159 (1979) 213.
[25] J. Smit and J. Vink, Nucl. Phys. \textbf{B284} (1987) 234.
[26] A. Smilga, Phys. Rev. \textbf{D 46} (1992) 5598.
[27] Ukawa, Phys. Rev. Lett. \textbf{72} (1994) 3448.
[28] T. Schäfer, E. V. Shuryak, \textit{Glueballs and Instantons}, SUNY-NTG preprint.
[29] E. V. Shuryak, Nucl. Phys. \textbf{B302}, 559,574,599 (1988)
[30] E. Shuryak, Nucl. Phys.\textbf{B319}, 511,521 (1989); \textbf{B328}, 85,102 (1989)
[31] E.V. Shuryak and J.J.M. Verbaarschot, Nucl. Phys. \textbf{B364} (1991) 255.
[32] D. I. Diakonov and V. Yu. Petrov, Nucl. Phys. \textbf{B245}, 259 (1984); D. I. Diakonov, V. Yu. Petrov, Nucl. Phys. \textbf{B272}, 457 (1986).
[33] M. A. Nowak, J. J. M. Verbaarschot and I. Zahed, Nucl. Phys. \textbf{B324}, 1 (1989)
[34] J.J.M. Verbaarschot, Nucl. Phys. \textbf{B362} (1991) 33.
[35] E.V. Shuryak and J.J.M. Verbaarschot, Phys. Rev. Lett. \textbf{68} (1992) 2576.
[36] A.V. Yung, Nucl. Phys. \textbf{B297} (1988) 47.
[37] D. I. Diakonov, V. Yu. Petrov, Nucl. Phys. (1993).
[38] K. Langfeld and H. Reinhardt, Scale anomaly induced instanton interaction (1994).
[39] P. Di Vecchia and G. Veneziano, Nucl. Phys. \textbf{B171} (1980) 253.
[40] D.I. Diakonov and V.Yu. Petrov, Leningrad Preprint LNPI-1153, 1986.
[41] M.A. Nowak, J.J.M. Verbaarschot and I. Zahed, Phys. Lett. \textbf{B228} (1989) 251; R. Alkofer, M.A. Nowak, J.J.M. Verbaarschot and I. Zahed, Phys. Lett. \textbf{B233} (1989) 205.
[42] C. G. Callan, R. Dashen and D. J. Gross, Phys. Rev. \textbf{D17}, 2717 (1978),
[43] R. Shrock, \textit{Lattice Yukawamodels} in \textit{Quantum Fieldson the Computer}, ed. M. Creutz, World Scientific 1992.
[44] E.M. Ilgenfritz, Habilitation Leipzig, 1988.
Figure Captions

Fig. 1. The integrated topological charge in the Debije cloud of an anti-instanton in a slice of length $l_4$ in the 4 direction of total length $2L$. The results are for $N_c = 3$ and two flavors with masses (in units of $fm^{-1}$) as given in the label of the figure.

Fig. 2. The pseudoscalar correlator $K_P(l_4)$ (upper figure) and the scalar gluonic correlator $K_S(l_4)$ (lower figure) as a function of the length of the slice, $l_4$, in the 4 direction of total length $2L$. The full line is for randomly positioned instantons and the dashed curves represent results of a fit. All result in this figure are for two colors and one or two massless flavors.

Fig. 3. The mass dependence of the pseudoscalar topological correlator for three colors and two flavors of equal mass (in units of $fm^{-1}$) given in the label of the figures. For further explanation we refer the the caption of Fig. 2.

Fig. 4. The pseudoscalar correlator $K_P(l_4)$ (upper figure) and the scalar gluonic correlator $K_S(l_4)$ (lower figure) as a function of the length $l_4$ of the subvolume for $N_c = 3$, $N_f = 3$ and $m_u = m_d = 10MeV$ and $m_s = 150MeV$. Further explanation can be found in the caption of Fig. 2.

Fig. 5. The mass dependence of the scalar topological correlator, $K_S(l_4)$, for three colors and two flavors of equal mass (in units of $fm^{-1}$) given in the label of the figures. For further explanation we refer the the caption of Fig. 2.