

**Instanton contributions to the low-lying hadron mass spectrum**

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The role of instanton-like objects in the QCD vacuum on the mass spectrum of low-lying light hadrons is explored in lattice QCD. Using overimproved stout-link smearing, tuned to preserve instanton-like objects in the QCD vacuum, the evolution of the mass spectrum under smearing is examined. The calculation is performed using a  $20^3 \times 40$  dynamical fat-link-irrelevant-clover (FLIC) fermion action ensemble with lattice spacing 0.126 fm. Through the consideration of a range of pion masses, the effect of the vacuum instanton content is compared at a common pion mass. While the qualitative features of ground-state hadrons are preserved on instanton-dominated configurations, the excitation spectrum experiences significant changes. The underlying physics revealed shows little similarity to the direct-instanton-interaction predictions of the instanton liquid model.

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**I. INTRODUCTION**

The instanton [1] is well known as a classical solution to the pure-gauge Yang-Mills equations. It has topological charge  $\pm 1$ , action  $8\pi^2/g^2$ , and is associated with a localized zero eigenmode of the Dirac operator. Various models exist for the QCD vacuum as composed purely of superpositions of these objects, and here we consider the random instanton liquid model (RILM) [2–7] as a point of comparison. Phenomenology constrains the RILM model parameters, including  $\rho_{\text{inst}} \approx 0.33$  fm for the average instanton size and  $n \approx 1$  fm $^{-4}$  for the pseudoparticle density.

Such a model vacuum generates approximate Dirac zero modes with definite chirality. A quark propagating via a zero mode changes its chirality. Thus, the masses of the pseudoscalar channels (the pion, and the diquark in the nucleon) have direct-instanton-induced contributions which are attractive and reduce their mass. By comparison, the rho as a vector meson has instanton contributions only at a higher level (analogous to a  $2\pi$  intermediate state). Similarly, the Delta has interactions only at the six-pseudoparticle level and higher [8–12].

We wish to determine what role the instantons present in the QCD vacuum of lattice QCD simulations play in the determination of hadron phenomenology. Starting from a Monte Carlo-generated calculation of QCD on the lattice, we filter out the short-distance gluonic interactions such that the underlying instanton degrees of freedom are revealed. We use overimproved stout-link smearing [13] to do this, and the merits of this approach are discussed in Sec. II.

Section III provides an overview of the lattice QCD simulation methods and associated parameters. It also describes our correlation matrix approach which enables

us to accurately determine both the ground-state hadron spectrum and the first radial excitations.

We will then examine the low-lying hadron spectrum as a function of smearing in Sec. IV, monitoring its evolution as the QCD vacuum progresses from having significant topological structure, most of it not instanton-like, through to being both instanton dominated and eventually sparse as nearby instanton–anti-instanton pairs annihilate. Conclusions are drawn in Sec. V.

**II. REVEALING INSTANTONS**

Early methods of smoothing short-distance fluctuations to reveal the underlying instanton degrees of freedom used cooling. This proceeds by replacing each link  $U_\mu(x)$  on the lattice with a new link such that the gluonic action is minimized. Unfortunately, this approach also tends to remove the topological configurations of interest from the lattice. This occurs due to the discretization error involved in minimizing the local action. Expanding the gluonic Wilson action in terms of a single-instanton solution, one finds [14]

$$S_{\text{inst}} = \frac{8\pi^2}{g^2} \left\{ 1 - \frac{1}{5} \left( \frac{a}{\rho} \right)^2 + O(a^4) \right\}. \quad (1)$$

Thus, the discretization error enables one to reduce the action by reducing the instanton size parameter  $\rho$ . Upon minimizing the action, instantons shrink. At sufficient cooling, they will become small enough that significant discretization errors will allow them to “fall through” the lattice.

It is possible, however, to include larger combinations of loops having different discretization errors. Coefficients can be chosen such that the  $O(a^2)$  error is canceled [15], giving the “improved” action. Unfortunately, this method still leads to a negative leading  $O(a^4)$  discretization error, and the same unwanted corrosion of topological objects.

Higher-order terms composed from combinations of larger loops can also be included in the action, but this requires increasing accuracy on the perturbative corrections to the improvement coefficients, typically estimated via the mean link of tadpole improvement.

Instead, one can adopt the approach of overimprovement [13,14] and express the action in terms of an improvement parameter  $\epsilon$ ,

$$S(\epsilon) = \beta \sum_x \sum_{\mu > \nu} \left\{ \frac{5-2\epsilon}{3} (1 - P_{\mu\nu}(x)) - \frac{1-\epsilon}{12} [(1 - R_{\mu\nu}(x)) + (1 - R_{\nu\mu}(x))] \right\}, \quad (2)$$

where  $P_{\mu\nu}(x)$  denotes 1/3 of the real trace of the clover average of the four plaquettes touching the point  $x$ , and similarly  $R_{\mu\nu}(x)$  denotes 1/3 of the real trace of the clover average of four  $2 \times 1$  Wilson loops. The choice of  $2 \times 1$  rectangles over the  $2 \times 2$  squares in Ref. [13] is in the interest of preserving locality and minimizing the number of links. The coefficients are chosen such that  $\epsilon = 1$  gives the unimproved Wilson action and  $\epsilon = 0$  provides an  $O(a^2)$ -improved action. We can also compare the behavior of the smearing algorithm to that provided by the Wilson or gradient flow, as in Ref. [16]. For  $\epsilon = 0$ ,  $N$  sweeps of stout-link smearing is equivalent to  $t = \alpha N$  for the Wilson flow time as long as the smearing parameter  $\alpha$  is sufficiently small. We use  $\alpha = 0.06$ , which is even smaller than the standard  $\alpha = 0.1$  for stout-link smearing.

A negative value for the  $\epsilon$  parameter will lead to a positive leading-order discretization error which inhibits the shrinking of instanton-like structures under smearing. However, a large negative value would cause instantons to grow under smearing. We use an  $\epsilon$  value of  $-0.25$ , as recommended in Ref. [13], providing the required stability with marginal discretization error. The effect of  $\epsilon$  is also studied in Sec. IV.

This scheme preserves instanton-like objects with a size parameter  $\rho$  greater than the dislocation threshold of  $1.97a$  [13]. Herein,  $a = 0.126$  fm, such that instantons of size  $\rho < 0.25$  fm will be removed under overimproved stout-link smearing [13]. However, this effect may be regarded as small. The scale dependence of the instanton action  $S_0 = 8\pi^2/g^2$  on the coupling constant  $g$  in the context of asymptotic freedom suppresses the presence of small instantons. A study of the instanton distribution within dynamical gauge fields with light dynamical quarks provides [17]  $\rho_{\text{inst}} = 0.415$  fm with the standard deviation of the distribution of instanton sizes of only 0.075 fm indicating a sharply peaked distribution with few small-size instantons.

An additional effect of smearing is that any smearing algorithm designed to suppress short-distance perturbative interactions from the gauge field will also tend to annihilate closely spaced instanton–anti-instanton pairs. As the effect

of this is mainly to reduce the pseudoparticle density, we expect a corresponding change in the quark condensate [4]. We will use this behavior of the smearing algorithm to examine the lattice QCD vacuum as it progresses from having significant topological structure, most of it not instanton-like, through to being both instanton dominated and sparse.

### III. SIMULATION METHODS

#### A. Correlation functions and the variational approach

The low-lying hadronic masses can be extracted from the lattice by analysis of their corresponding two-point correlation functions. This correlation function is defined as  $G_2(x) = \langle 0 | \chi(x) \bar{\chi}(0) | 0 \rangle$ , where  $\chi$  is the interpolating field corresponding to the hadron of interest. The correlation function, in momentum space, is then of the form

$$G_2(\vec{p}, t) = \sum_{\vec{x}} \exp(-i\vec{p} \cdot \vec{x}) \langle 0 | \chi(x) \bar{\chi}(0) | 0 \rangle. \quad (3)$$

Inserting a complete set of states,  $|B\rangle$ , and utilizing the translation operator, one obtains the Euclidean time correlator

$$G_2(\vec{p}, t) = \sum_B e^{-E_B(\vec{p})t} \lambda_B(\vec{p}) \bar{\lambda}_B(\vec{p}), \quad (4)$$

with  $\lambda_B(\vec{p}) = \langle 0 | \chi | B, \vec{p} \rangle$  describing the coupling of the state  $B$  with momentum  $\vec{p}$  to the operator  $\chi$  and  $E_B(\vec{p})$  the on-shell energy of the state.

The determination of the mass of the lowest-lying state is hampered by the tower of exponentials from excited-state contributions. Although these are suppressed by the factor  $e^{-E_B t}$ , it is often difficult to wait until a sufficiently large Euclidean time where all excited-state contaminations have vanished. Moreover, with broad fermion source smearings and narrow fermion sink smearings, excited states can enter with a negative weight and create false plateaus.

This problem is particularly challenging on smeared configurations. As we will see, hadronic excited states do not maintain a significant mass splitting from the ground-state hadrons, making the extraction of even the ground-state mass difficult.

The solution to the state isolation problem is now well established. One considers a matrix of correlation functions in a variational analysis [18–20]. The operators used to create the correlation functions can be chosen to have any form (as long as they have the correct quantum numbers). Different operators have different couplings  $\lambda_B$  to each state  $B$ , and one seeks linear combinations of the operators constructed to isolate each state of the spectrum.

The best approach for isolating a state within a tower of states excited by a particular interpolating field is to introduce differently sized covariantly smeared sources

and sinks [21–23]. Physical hadrons are extended objects, and a linear combination of Gaussian sources allows one to approximate the hadronic wave function [24]. This allows for a precise determination of ground-state properties. The suppression of excited states provides ground-state isolation early in Euclidean time. The approach also provides access to the excited states having the same spin and parity.

We solve the generalized eigenvalue problem for the matrix  $G_{ij}$  whose elements are the correlation functions generated from the operators  $\chi_i$  and  $\bar{\chi}_j$ , normalized at the fermionic source time. If  $\bar{\phi}^\alpha = u_j^\alpha \bar{\chi}_j$  is an operator constructed to isolate state  $\alpha$ , then the recurrence relation relating times  $t_0$  and  $t_0 + dt$ ,

$$G_{ij}(t_0 + dt)u_j^\alpha = e^{-E_\alpha dt}G_{ij}(t_0)u_j^\alpha, \quad (5)$$

can be used to construct a generalized eigenvalue equation for the right eigenvector  $u^\alpha$  and eigenvalue  $e^{-E_\alpha dt}$ :

$$G^{-1}(t_0)G(t_0 + dt)u^\alpha = e^{-E_\alpha dt}u^\alpha. \quad (6)$$

The reference times  $t_0$  and interval  $dt$  must be selected to lie within a region where the excited-state contributions are strong and not yet exponentially suppressed. However, some amount of Euclidean time evolution is helpful in reducing the number of states contributing significantly in the correlators to the dimension of the correlation matrix such that state isolation is achieved.

While the eigenvalues of the generalized eigenvalue equations depend strongly on the values of these variational parameters,  $t_0$  and  $dt$ , the associated eigenvectors are robust against this variation. A similar analysis can be done to obtain the left eigenvector  $v^\alpha$ , from which a state-projected correlator  $v_i^\alpha G_{ij}(t)u_j^\alpha$  can be constructed.

This correlator is insensitive to the variational parameters. In practice, a  $t_0$  value 1 or 2 time steps from the source accompanied by a  $dt$  value of 2 or 3 lattice time steps provides good eigenstate isolation in the projected correlator. One can then apply standard analysis techniques using the covariance matrix-based  $\chi^2$  per degree of freedom to carefully identify the Euclidean time regime dominated by a single eigenstate.

## B. Simulation methods and parameters

Previous works in this vein [25–28] were considered in the mid to late 1990s. While they often considered the quenched approximation, a greater concern is the use of standard cooling algorithms based on the Wilson gauge action.

As discussed in Sec. II, this algorithm rapidly destroys the instanton-like topological structures that one is attempting to study. In this case, the final smeared configuration is much closer to a dilute instanton gas than to an instanton liquid.

The calculations presented herein are performed on an ensemble of 76 two-flavor  $20^3 \times 40$  gauge field configurations generated using dynamical fat-link-irrelevant-clover (FLIC) fermions [29–33], with lattice coupling  $\beta = 3.94$  and an  $SU(3)$ -flavor symmetric hopping parameter  $\kappa = 0.1324$ , providing  $m_\pi = 540$  MeV. The lattice spacing associated with the string tension is  $a = 0.126$  fm, providing a spatial extent of 2.52 fm. As a smearing sweep is a local short-distance effect that does not affect the string tension, we consider the lattice spacing to be unaltered under a smearing sweep. Cumulative smearing sweeps do affect long-distance physics, and we will examine this effect in the following section.

The smearing of the gauge field is performed using overimproved stout-link smearing [13] with  $\epsilon = -0.25$  and an isotropic smearing parameter  $\alpha_{\text{sm}} = 0.06$ , smaller than the typical value [34] of 0.10.

Valence quark propagators are calculated via the FLIC fermion action at multiple  $\kappa$  values. The boundary conditions are periodic in the spatial dimensions, and fixed in the Euclidean time dimension. The fermionic source is inserted away from the boundary at  $t = 10$ , sufficient to avoid artifacts associated with the boundary. In constructing a basis for our variational approach to isolating states, we use gauge-invariant Gaussian smeared [35] fermion sources. The smearing procedure is

$$\psi_i(x, t) = \sum_{x'} F(x, x') \psi_{i-1}(x', t), \quad (7)$$

where

$$F(x, x') = (1 - \alpha) \delta_{x, x'} + \frac{\alpha}{6} \sum_{\mu=1}^3 [U_\mu(x) \delta_{x', x+\hat{\mu}} + U_\mu^\dagger(x - \hat{\mu}) \delta_{x', x-\hat{\mu}}], \quad (8)$$

and the parameter  $\alpha = 0.7$  is used in our calculation. After repeating the procedure  $N_{\text{sm}}$  times on a point source, the resulting smeared fermion field is

$$\psi_{N_{\text{sm}}}(x, t) = \sum_{x'} F^{N_{\text{sm}}}(x, x') \psi_0(x', t). \quad (9)$$

We consider  $N_{\text{sm}} = 10, 25, 50, 100$ , and 150 sweeps in constructing effective correlation-matrix bases.

## IV. RESULTS

### A. Gluonic observables

We begin by examining the effect of stout-link smearing on the action of our gauge-field ensemble. Figure 1 displays the evolution of the action as a function of the number of smearing sweeps. For our choice of  $\epsilon = -0.25$ , after only 10 sweeps of smearing, the action has dropped to one tenth of its initial value. The majority of the short-distance

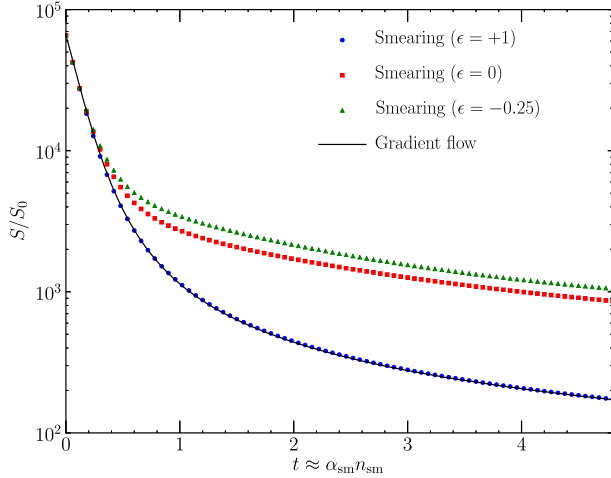


FIG. 1 (color online). The evolution of the action for a typical configuration under various methods of smearing.  $\epsilon = 1$  is the Wilson action, and  $\epsilon = 0$  corresponds to the  $\mathcal{O}(a^2)$ -improved action. The action under overimproved smearing ( $\epsilon = -0.25$ ) lies above either of these as required. With the identification  $t = \alpha_{\text{sm}} n_{\text{sm}}$  using our value of  $\alpha_{\text{sm}} = 0.06$ , numerical integration of the Wilson flow agrees with smearing using the Wilson action. The highest level of smearing considered in the following sections (60 sweeps) is equivalent to a Wilson flow time of  $t = 3.6$ . An approximation to the instanton density can be retrieved by dividing by the lattice volume  $V \approx 81 \text{ fm}^4$ .

interactions are removed within the first few iterations of smearing. It takes another 50 sweeps of smearing for the action to reduce by another order of magnitude. The Wilson flow is also shown for comparison of smearing extent. We will focus on ensembles following 10, 20, 40, and 60 sweeps of smearing; these correspond to Wilson flow times of 0.6, 1.2, 2.4, and 3.6, respectively.

In Fig. 2, the static quark potential, determined from the Wilson loop, is shown for configurations at various levels of smearing. The attractive Coulomb-potential behavior at small  $r$  is lost rapidly under smearing as the algorithm removes short-distance interactions. The fit is a third-order Padé approximant constrained by the short-distance behavior  $V \rightarrow V_{\text{free}} = 0$  and the long-distance behavior of a linearly rising potential. It has the form

$$V(r) = \frac{a_1 r + a_2 r^2 + a_3 r^3}{b_0 + b_1 r + r^2}. \quad (10)$$

The large  $r$  slope of the potential reflects the approximate invariance of the string tension and associated lattice spacing. Best-fit parameters are summarized in Table I.

For sufficiently large  $r$ , the parameter  $a_3$  is equivalent to the string tension  $\sigma$ , and we note it remains almost constant under moderate levels of smearing. This differs significantly from the behavior reported in Ref. [25], where the string tension was reduced to only 27% of its original value after 25 sweeps of the unimproved cooling algorithm.

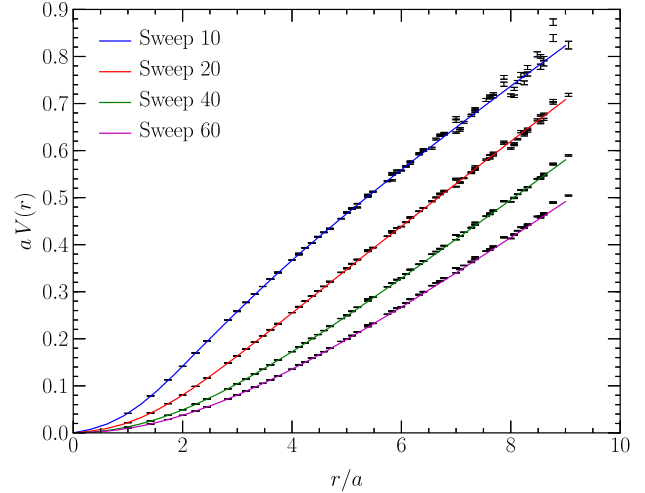


FIG. 2 (color online). The evolution of the static quark potential under various levels of overimproved stout-link smearing.

This also differs from the theoretical prediction of the instanton liquid model, which was shown to generate a string tension [36], but with a value much smaller than the physical value. The overimproved stout-link smearing algorithm tuned specifically to preserve instanton-like structure in the gauge field configurations retains the long-distance string tension remarkably well.

The process of stout-link smearing is expected to remove the short-distance physics up to an effective radius [37] which may be parametrized as

$$R = a(c\rho_{\text{sm}}N_{\text{sw}})^{1/2} \quad (11)$$

under the random-walk hypothesis. The coefficient  $c$  is a proportionality constant determined [37] to be  $c = 6.15(3)$ . The smearing radii for our selected values of  $N_{\text{sw}} = 0, 10, 20, 40, 60$  are  $R/a = 0, 1.9, 2.7, 3.8, 4.7$  respectively. While this explains the preservation of the string tension observed in Fig. 2 and Table I, one needs to examine the extent to which an ensemble of instantons has been isolated in the QCD vacuum.

The instanton content of the vacuum under the same overimproved stout-link smearing algorithm selected herein was also studied in Ref. [38]. To examine the extent

TABLE I. The best-fit parameters for the Padé of Eq. (10) fit to the lattice QCD results for the static quark potential illustrated in Fig. 2. Uncertainties in the parameters are determined from a single-elimination jackknife analysis.

Sweep	$a_1$	$a_2$	$a_3$	$b_0$	$b_1$
10	0.093(2)	0.01(1)	0.082(1)	4.7(2)	-1.22(5)
20	0.062(1)	0.020(4)	0.084(1)	6.4(2)	0.22(3)
40	0.035(1)	0.212(4)	0.081(1)	21.4(3)	3.28(5)
60	0.02(5)	0.384(1)	0.073(1)	42(1)	5(1)



to which the nontrivial topology identified on the lattice is consistent with instantons, two measures of the local maxima of the action density found on representative configurations were taken and compared to the classical instanton solution. The instanton size is measured by fitting the profile of the action density in a  $(2a)^4$  hypercube surrounding the position of the local maximum to the classical instanton action density

$$S_0(x) = \xi \frac{6}{\pi^2} \frac{\rho^4}{((x - x_0)^2 + \rho^2)^4}. \quad (12)$$

Here  $\xi$ ,  $\rho$  and  $x_0$  are fit parameters, noting that  $x_0$  is not restricted to a lattice site. The parameter  $\xi$  is introduced, as lattice topological objects often have a higher action than classical instantons. We wish to determine the size,  $\rho$ , by using the shape of the action density around the local maximum, rather than the height. Considering the relative rms deviation over the  $3^4$  hypercube of points surrounding the local maximum,  $\sqrt{\frac{1}{V-1} \sum_{x \in V} (S_0(x) - \bar{S})^2} / \bar{S}$ , we find Eq. (12) fits the data with a typical percentage deviation of 10%. This deviation decreases as the gauge fields are smeared.

We can then compare the size of instanton candidates to the value of the topological charge at the center of an (anti-)instanton in the context of the classical instanton relationship

$$q(x_0) = Q \frac{6}{\pi^2 \rho^4}, \quad (13)$$

where  $Q = \mp 1$  for an (anti-)instanton.  $q(x_0)$  at the fitted values of  $x_0$  are found using linear interpolation from neighboring hypercubes to find an extremum inside the hypercube containing  $x_0$ .

Fig. 3, reproduced from Ref. [38], displays the values found on a smoothed lattice at various smearing levels and compares the distribution with the classical relationship of Eq. (13), illustrated by the curves. The degree to which fitted results concur with Eq. (13) provides insight into the extent to which the topology of the gluon fields resembles an ensemble of instantons.

At low levels of smearing we expect to fit a large number of local maxima which are not associated with the nontrivial topology of instantons—local maxima of the action corresponding to noise. At 10 sweeps, the number of instanton candidates is large and distributed with sizes greater than the dislocation threshold of  $\sim 2$  through 8 lattice units. There is little correlation to the predicted charge lines of Eq. (13). However, this quickly changes as the number of smearing sweeps increases, eventually leading to a very close approximation to Eq. (13). In this case the distribution reflects an ensemble of topological objects approximating classical instanton solutions. In principle, there are also exactly (anti-)self-dual classical solutions with nontrivial holonomy (i.e. calorons) which

wrap around the temporal extent of the lattice [39–42]. When the spatial extent (the separation of the monopole constituents) of these objects is much less than the time extent of the lattice, the action and charge density near their peak approaches the single-instanton solution while still differing in the low-field region. Such objects are thus a possible alternative interpretation to BPST instantons for the local maxima found. This possibility has not been checked, and goes beyond the scope of the current investigation.

The number of instanton candidates steadily decreases with smearing through the process of neighboring instanton–anti-instanton annihilation. By 100 sweeps the number of instanton candidates has been thinned to the point that they are usually well separated, and thus the annihilation of instanton pairs is very slow. We examine the region of interest where one has an ensemble of overlapping instantons and bracket this regime with configuration ensembles having 20, 40 and 60 sweeps of smearing. Using the number of local maxima found in the action density, we find pseudoparticle densities of 7.9, 3.6, and 2.4 fm<sup>-4</sup> for 20-, 40-, and 60-sweep ensembles, respectively.

## B. Gell-Mann-Oakes-Renner relation

We commence with an investigation of the pion mass and consider the standard pseudoscalar interpolating field  $\chi = \bar{u}^a(x) \gamma_5 d^a(x)$ . Our first consideration is the extent to which the Gell-Mann-Oakes-Renner [43] relationship between the squared pion mass and the quark mass ( $m_u = m_d = m_q$ ),

$$m_\pi^2 = -\frac{2\langle q\bar{q} \rangle}{f_\pi^2} m_q, \quad (14)$$

is maintained on the smeared ensembles. We consider a wide range of hopping parameter values,  $\kappa$ , and examine the relationship between the squared pion mass and  $1/\kappa \propto m_q$ .

Unlike the case of center-vortex removal [44], we find a linear relationship at all levels of smearing. This enables the standard approach of dealing with the additive renormalization of the quark mass in Wilson-like fermion formulations such as the FLIC fermion action considered herein. The critical value of the hopping parameter,  $\kappa_{\text{cr}}$ , where the pion mass vanishes, is determined by linearly extrapolating  $m_\pi^2$  as a function of  $1/\kappa$  to zero. The additively renormalized quark mass is then provided by the standard relation

$$m_q = \frac{1}{2a} \left( \frac{1}{\kappa} - \frac{1}{\kappa_{\text{cr}}} \right). \quad (15)$$

The value of  $\kappa_{\text{cr}}$  observed depends significantly on the first few sweeps of smearing. Its deviation from the tree-level value of  $1/8$  is an indication of the additive renormalization of the quark mass induced by the explicitly broken chiral symmetry of the Wilson action. As smearing removes the perturbative physics which acts to renormalize  $\kappa_{\text{cr}}$  away

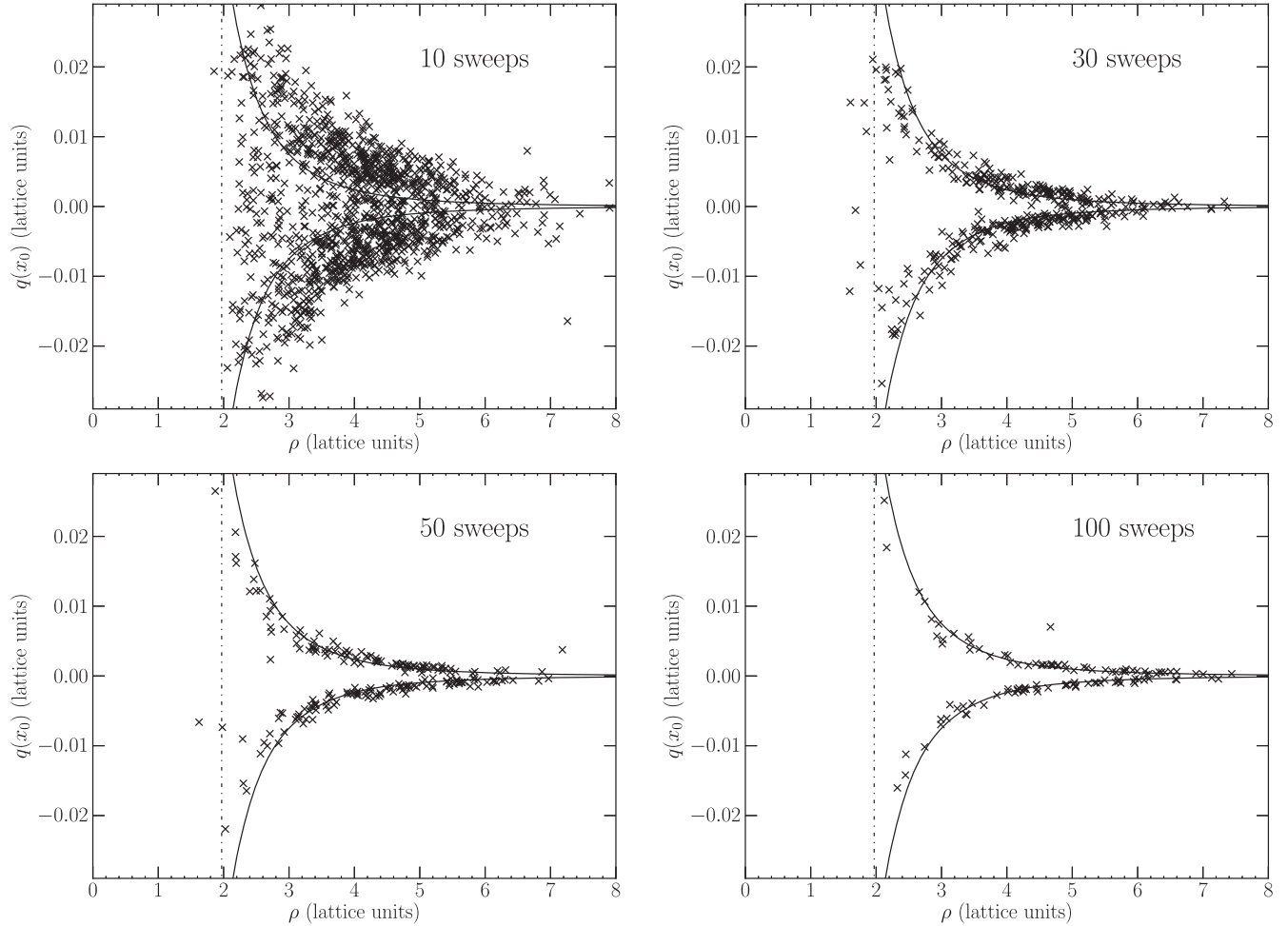


FIG. 3. Instanton content of a single representative gauge field configuration under the overimproved stout-link smearing algorithm at 10, 30, 50 and 100 sweeps of smearing, reproduced using data from Ref. [38]. At each smearing level, the gauge action  $S/S_0 = 2099, 445, 252, 130$ ; topological charge  $Q = -9.45, -7.36, -6.38, -6.02$ , and approximate instanton number (determined only by the number of candidates)  $n = 1222, 400, 214, 116$ . The values of the instanton size,  $\rho$ , found by fitting lattice maxima of the action to the classical instanton action density, are plotted as crosses, against the topological charge at the center,  $q(x_0)$ . The results are compared to the theoretical relationship between the instanton radius and topological charge at the center (solid lines), and the dislocation threshold of the algorithm,  $1.97a$  (dash-dotted line). The pseudoparticle densities underlying the gauge fields considered remain higher than the phenomenologically assumed value of  $\approx 1 \text{ fm}^{-4}$ , which would correspond to an instanton number of  $\approx 80$ .

from its tree-level value, one observes a return of  $\kappa_{\text{cr}}$  to 0.125. Similarly, the mean link, provided by the fourth root of the average plaquette, approaches 1. For example, after 10 sweeps of smearing, the original value of  $\kappa_{\text{cr}} = 0.135$  becomes 0.126, and  $u_0 = 0.86$  subsequently exceeds 0.995. The latter result indicates that the multiplicative renormalization of the quark mass in the smeared ensembles is negligible.

Our results are illustrated in Fig. 4. The Goldstone nature of the pion is indeed retained. However, there is a significant variation in the slope of the linear relation that reflects an important change in the manner in which the quark mass manifests itself in the interacting field theory.

The slope,  $-2\langle q\bar{q} \rangle / f_\pi^2$ , can be regarded as an indicator of the level of instanton preservation under smearing. Figure 5 illustrates its evolution under smearing. In an instanton

model, the quark condensate is proportional to  $\sqrt{n}$ , where  $n$  is the instanton density. Thus, it is understandable that the slope reduces under smearing as instanton–anti-instanton pairs are annihilated.

In comparing results from different levels of smearing, one can choose to keep the bare mass  $m_q$  fixed, or to keep  $m_\pi$  fixed as a measure of the renormalized quark mass. We choose the latter as providing the more physical relationship between ensembles with differing levels of smearing. It also enables a connection to the original unsmeared ensemble results.

### C. Ground-state hadrons

We now consider the remaining lowest-lying light hadrons with nonvanishing masses in the chiral limit: the rho meson, the nucleon, and the Delta baryon. We use the

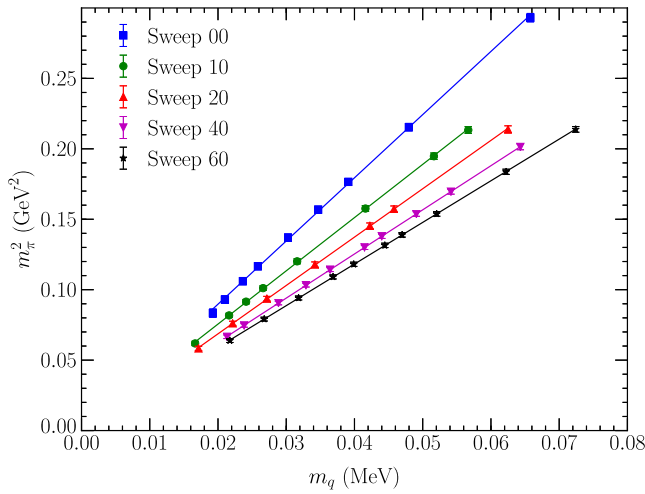


FIG. 4 (color online). The squared pion mass is plotted as a function of the Wilson quark mass of Eq. (15). Results are provided for the original configurations (Sweep 00) and for the ensembles following various levels of overimproved stout-link smearing as indicated.

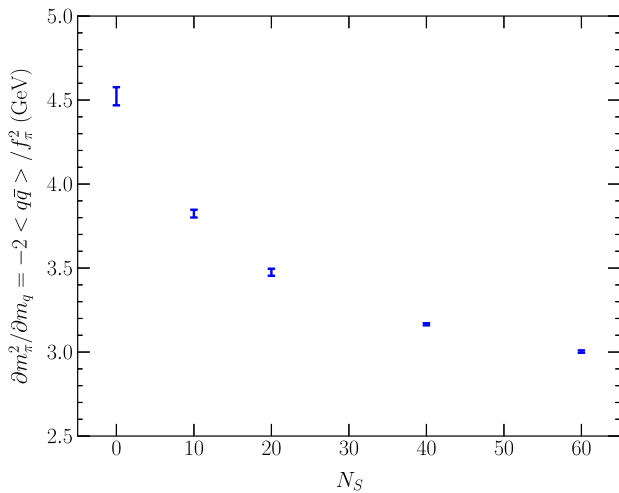


FIG. 5 (color online). The slope of the Gell-Mann-Oakes-Renner relation as a function of smearing.

standard interpolating fields for the  $\rho$  [ $\bar{u}^a \gamma_\mu d^a$ ], the nucleon [ $\epsilon^{\text{abc}}(u^{T a} C \gamma_5 d^b) u^c$ ], and the  $\Delta$  [ $\epsilon^{\text{abc}}(u^{T a} C \gamma_\mu u^b) u^c$ ], and construct a  $4 \times 4$  correlation matrix. A combination of Gaussians with  $N_{\text{sm}} = 25, 50, 100, 150$  was chosen to isolate states on the less smeared configurations ( $N_s < 40$ ). For the more heavily smeared configurations, the smoother background causes the process of source smearing to be more efficient—the same number of smearing sweeps gives a larger source. Thus, the  $N_{\text{sm}} = 100$  and  $N_{\text{sm}} = 150$  sources became too similar in shape for any linear combination of them to resolve different states. Thus, for these configurations ( $N_s = 40, N_s = 60$ ), the basis  $N_{\text{sm}} = 10, 25, 50, 100$  was chosen.

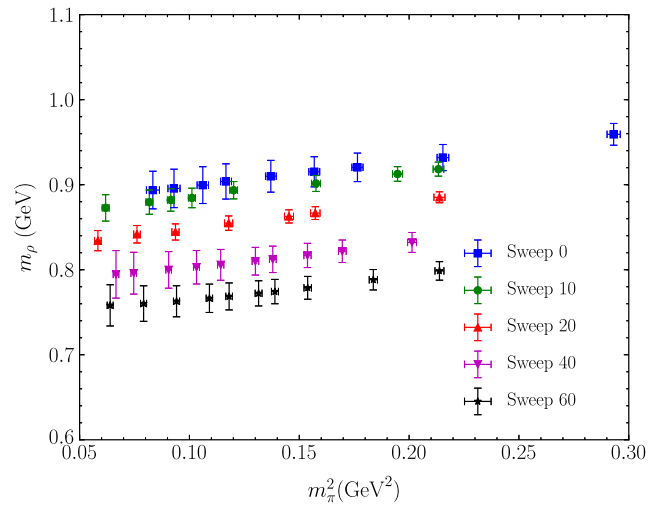


FIG. 6 (color online). Quark-mass dependence of the rho-meson mass for various levels of smearing.

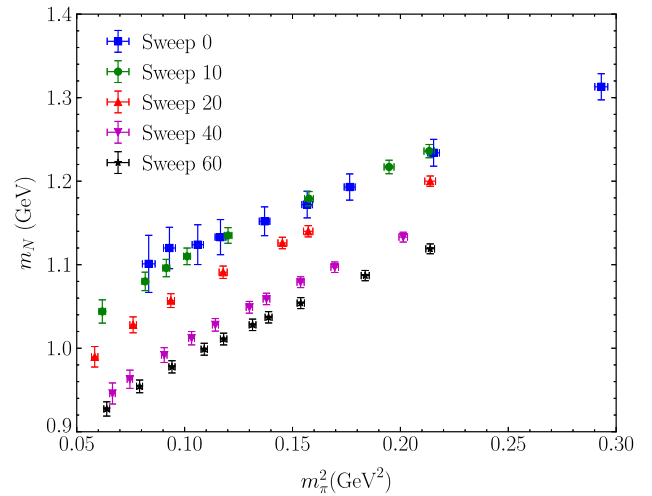


FIG. 7 (color online). Quark-mass dependence of the nucleon mass for various levels of smearing.

As illustrated in Figs. 6–8, the hadron masses display a common trend of reduction as the underlying instanton content of the vacuum is eroded through pair annihilation under smearing. Only subtle changes in the pion-mass dependence of the hadron masses are observed.

However, an important difference between these hadronic observables and gluonic observables is apparent. While gluonic observables such as the action and the short-distance potential undergo rapid transitions during the first few sweeps of smearing, these hadronic observables display very little change over the first 10 sweeps. One can conclude that the rapid loss of action density in the first few sweeps of cooling is not connected to the low-lying hadron masses in a significant manner. Rather, it is the loss of closely spaced instanton–anti-instanton pairs over more extensive smearing extents that gives rise to a

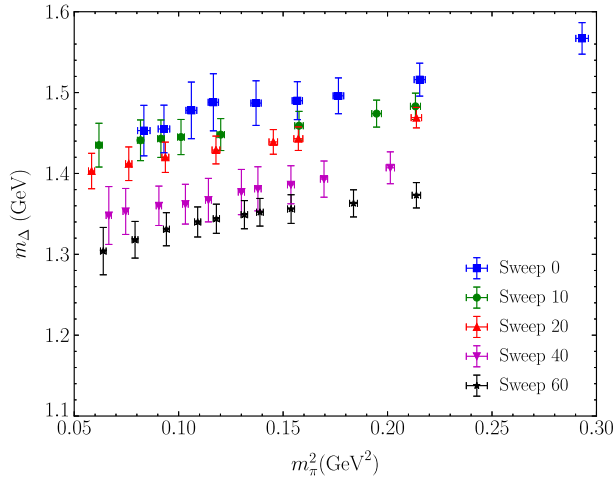


FIG. 8 (color online). Quark-mass dependence of the  $\Delta$  mass for various levels of smearing.

loss of dynamical mass generation and lower-lying hadron masses.

However, we emphasize, the pion is different. At larger values of the quark mass, the pion mass displays a more rapid transition over the first few sweeps as reported in Fig. 4. This behavior contrasts that of the  $\rho$ ,  $N$  and  $\Delta$ , where the change in the hadron mass is relatively insensitive to the quark mass.

To perform a more quantitative examination of these hadron masses, we interpolate the results to a common pion mass of 300 MeV and increase the statistical sample size by calculating eight fermionic sources (shifting by a quarter of the temporal extent, and by half the spatial extent in each direction) per configuration for a total of 608. We also consider an interpolation to  $m_\pi = 400$  MeV to expose any sensitivity to our selection of a comparison point. We note that for  $m_\pi = 300$  MeV,  $m_\pi L \sim 4$  such that finite-size effects are unlikely to affect the results in a significant manner.

Figures 9 and 10 report the results. While the hadron masses show a decline under smearing, we note that this decline is uniform for the  $N$  and  $\Delta$ . The mass splitting  $M_\Delta - M_N$  is invariant under smearing.

This invariance is interesting in the context of an instanton model where a strong attractive contribution to the nucleon mass originates from the interaction of the scalar diquark component with a single instanton or with a pair of an instanton and an anti-instanton (in the sum-rule context, the single-instanton contribution is necessary to stabilize the correlator) [10,45,46]. This contribution is necessarily large in typical models in order to replicate the observed nucleon-Delta mass splitting. In contrast, the lowest-order contribution to the Delta requires twice as many zero-mode contributions, and the instanton contribution to the mass is therefore higher order in  $n/V$ . In the current investigation, once the ultraviolet interactions have

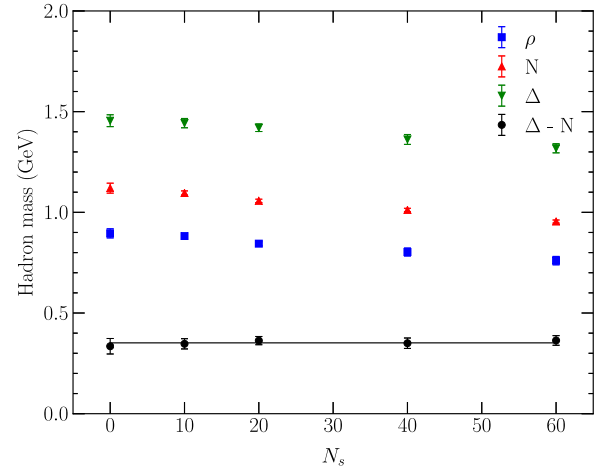


FIG. 9 (color online). Hadron masses, interpolated to a common pion mass of 300 MeV, are illustrated as a function of the number of smearing sweeps,  $N_s$ . The nucleon-Delta mass splitting,  $M_\Delta - M_N$ , is also illustrated. A fit of this splitting to a constant illustrates the invariance of the nucleon-Delta mass splitting to a thinning of the (anti-)instanton density.

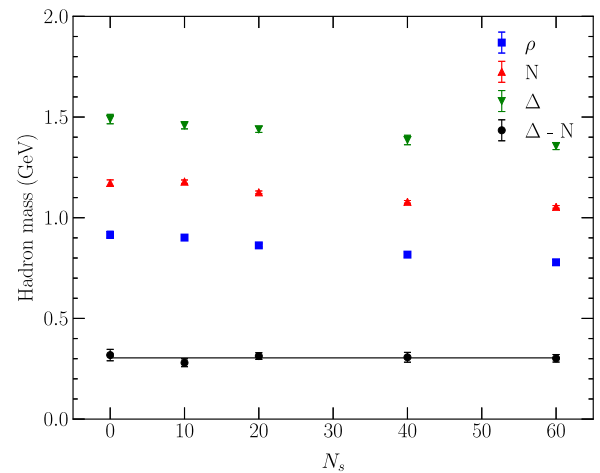


FIG. 10 (color online). Hadron masses, interpolated to a common pion mass of 400 MeV, are illustrated as a function of the number of smearing sweeps,  $N_s$ . A fit of the nucleon-Delta mass splitting,  $M_\Delta - M_N$ , to a constant illustrates the invariance of the nucleon-Delta mass splitting to a thinning of the (anti-)instanton density.

been suppressed under smearing, the main change to the gauge fields under further smearing is the annihilation of adjacent instanton-anti-instanton pairs. As the instanton-based model experiences a reduction in the scalar diquark attraction in the nucleon, it predicts a narrowing of the nucleon-Delta mass splitting under smearing. However, this is not observed. Figures 9 and 10 display a nucleon-Delta mass splitting that is invariant under smearing. Thus, the simple direct-instanton effect cannot be responsible for the lightness of the nucleon compared to the Delta.



In summary, the nucleon and Delta masses decrease under overimproved stout-link smearing. The reduction is of the order of 10% of their original masses after 60 sweeps of smearing. However, the mass splitting between them is insensitive to the loss of instanton pairs under smearing. Their mass splitting remains constant within error. The loss of instanton-induced scalar-diquark attraction in the nucleon predicted by the simple direct-instanton effect is not apparent. Although the majority of the hadron mass can be considered as generated by instanton interactions, this hadron-instanton interaction is not described using the 't Hooft interaction from a single instanton pair.

It is important to place this modern analysis in the context of an early analysis [25] that reported results consistent with the instanton model prediction. This early study considered smaller  $16^3 \times 24$  lattices with an uncooled lattice spacing of 0.168 fm. The ensemble consisted of only 19 gauge configurations, and the hadron masses on the cooled ensembles were fitted using their dispersion relation, because the statistical variation was too large on the cooled configurations to use the asymptotic behavior of  $e^{-mt}$ . The associated large discretization errors combined with unimproved cooling led to the rapid reduction of both ultraviolet physics and instanton content. Individual instantons are destroyed under unimproved cooling, leading to a rapid loss of gauge field dynamics. Using the nucleon mass to reset the lattice spacing after cooling, the Delta was found to be “too light.” The present analysis suggests that this loss of mass splitting reflects a loss of gauge field dynamics such that the nucleon and Delta simply become degenerate. In other words, the dynamics responsible for splitting them has been destroyed under unimproved cooling.

In contrast, the invariant mass splitting observed in the present analysis occurs in the context of declining nucleon and Delta masses. As a result, the Delta-nucleon mass ratio actually increases under smearing as illustrated in Fig. 11. While good agreement with the physical ratio of 1.31 is observed at small numbers of smearing sweeps, the Delta is “too heavy” at 60 sweeps of smearing when measured relative to the nucleon mass.

#### D. Excited states

Our use of the correlation matrix method to cleanly isolate the lowest-lying states presented thus far has the additional advantage that we are able to examine the behavior of excited states under smearing. To the best of our knowledge, this is the first examination of the role of instanton degrees of freedom in describing the radial excitations of hadrons.

Figures 12–14 illustrate the very different behavior of hadronic excitations under smearing. The variation in mass is not at the level of the 10% observed for ground states, but is of the order of 30%. Moreover, a significant mass drop is

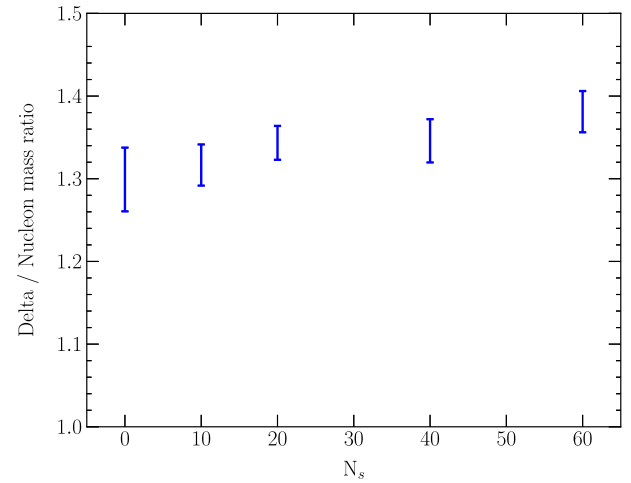


FIG. 11 (color online). The dependence of the  $\Delta/N$  mass ratio evaluated at  $m_\pi = 300$  MeV on the number of smearing sweeps. The ratio increases with smearing, reflecting a constant mass splitting in the context of decreasing baryon masses due to a thinning of the (anti-)instanton density.

observed for as few as 10 sweeps of smearing, signaling an important role for ultraviolet physics.

We note that the excited states at 40 sweeps of smearing do not follow the monotonic trend set by the other smearing levels. We believe these energies are affected by nearby states that are not adequately accommodated in the  $4 \times 4$  correlation matrix considered, giving rise to a superposition of excited states in the reported results. While we include them here for completeness, we will set them aside for the remainder of the discussion.

As for the ground states, we interpolate the hadron masses to common pion masses of 300 and 400 MeV. Their dependence on the number of smearing sweeps is illustrated in Figs. 15 and 16. While the ground-state hadrons

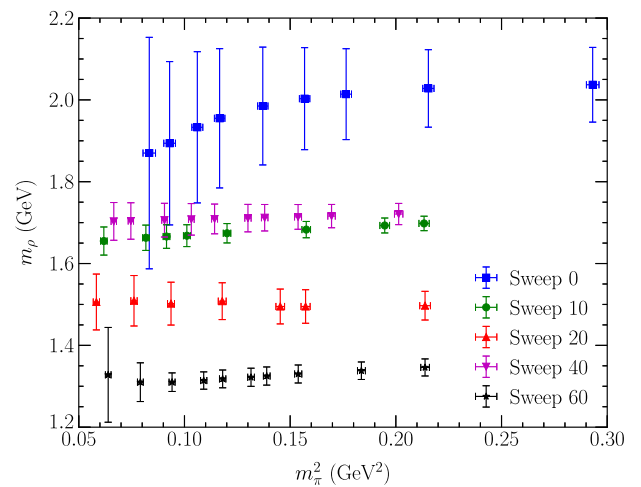


FIG. 12 (color online). Quark-mass dependence of the first-excited-state energy of the rho meson observed in our correlation-matrix analysis for various levels of smearing.

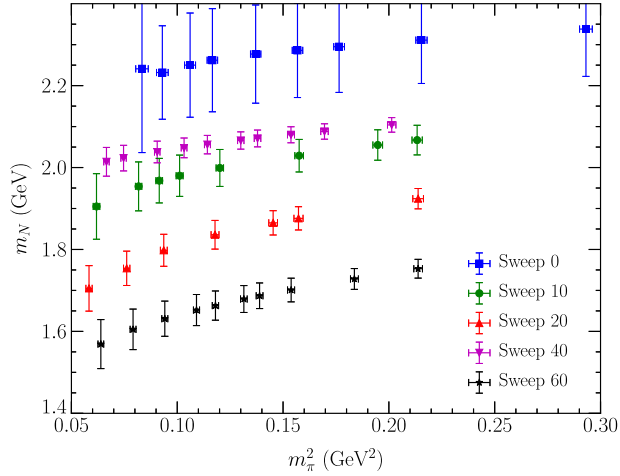


FIG. 13 (color online). Quark-mass dependence of the first-excited-state energy of the nucleon observed in our correlation-matrix analysis for various levels of smearing.

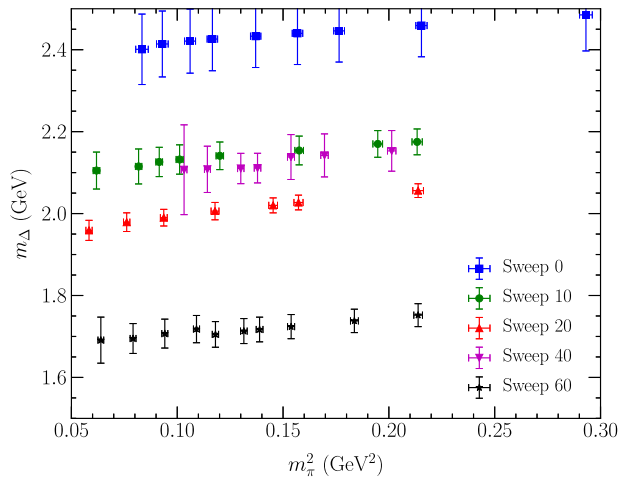


FIG. 14 (color online). Quark-mass dependence of the first-excited-state energy of the Delta observed in our correlation-matrix analysis for various levels of smearing.

remain qualitatively unchanged under smearing, the excited states decrease in mass significantly. Continued smearing leads to a significant decline in the excitation energy, again emphasizing an important role for instanton degrees of freedom in generating the excitation spectrum.

An analysis of the associated eigenvectors for the excited states indicates that these states have the expected single-node structure of a radial excitation in their wave function. The node is generated through a superposition of broad and narrow Gaussian smeared sources with opposite signs.

### E. Nonrelativistic quark model consideration

An interesting question is the extent to which our results reported in Figs. 15 and 16 can be described by a simple constituent quark model, drawing on the change of the static quark potential examined in Fig. 2.

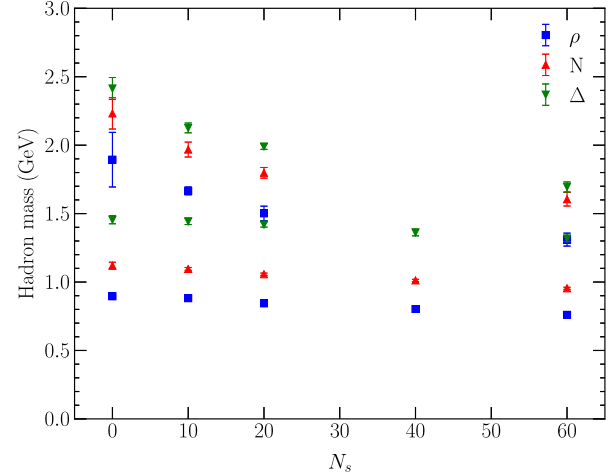


FIG. 15 (color online). The observed energies of the first excited states of our correlation matrix analysis are interpolated to a common pion mass of 300 MeV and plotted as a function of the number of smearing sweeps,  $N_s$ , to reveal the role of instanton degrees of freedom in generating the spectrum of excited states. The ground-state masses are also replotted for comparison.

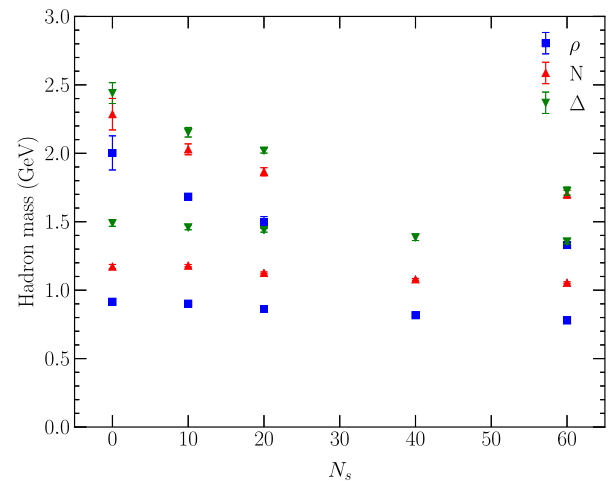


FIG. 16 (color online). The observed energies of the first excited states of our correlation matrix analysis are interpolated to a common pion mass of 400 MeV and plotted as a function of the number of smearing sweeps,  $N_s$ , to reveal the role of instanton degrees of freedom in generating the spectrum of excited states. Again, the ground-state masses are shown for comparison.

Here we consider the  $\rho$  meson. Using our fits to the static quark potential illustrated in Fig. 2, we solve the Schrödinger equation using a fixed constituent quark mass of 400 MeV and boundary conditions emulating the periodic lattice condition of the spatial volume.

As displayed in Fig. 17, this naive model predicts a much faster decrease in the ground-state mass than we observe in the lattice calculation. Moreover, the excited-state mass is maintained better than the ground-state mass under smearing. This qualitative difference allows us to conclude that a

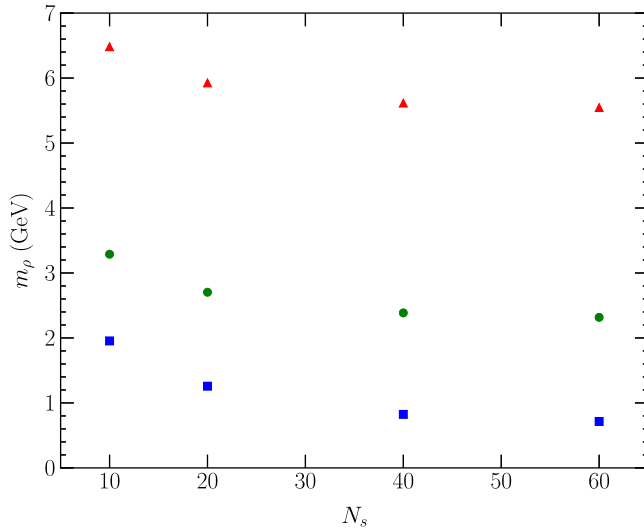


FIG. 17 (color online). Ground-state, first-excited-state, and second-excited-state masses of the  $\rho$  meson from a nonrelativistic quark model calculation based on the static quark potential fits illustrated in Fig. 2. Masses may be shifted vertically by introducing a constant into the potential.

simple modification of the potential energy between constituent quarks is insufficient to capture the essence of the modification of the QCD vacuum under smearing.

## V. CONCLUDING REMARKS

The light hadron spectrum has been examined in lattice QCD where the vacuum is altered using the overimproved stout-link smearing algorithm designed to retain separated instantons. The change in the ground-state hadron masses of the  $\rho$ ,  $N$  and  $\Delta$  is of the order of 10%, indicating that

almost all of the mass is generated by topological structures similar to instantons.

However, the difference between the Delta and nucleon masses is insensitive to smearing and the associated thinning of (anti-)instantons on the lattice. Even though the smearing process destroys topology by pairwise annihilation, the anticipated attractive contribution to the nucleon mass from the scalar-diquark direct-instanton interaction does not weaken during this process. This indicates that direct-instanton-induced effects are not the dominant contribution to the hadronic masses.

Similarly, simple quark model phenomenology differs from the results observed on the lattice. A deeper understanding of the underlying mechanisms of QCD could be obtained through the operator product expansion of two-point hadron correlation functions. The evolution of vacuum condensates under smearing could be examined, and the impact of this evolution on the spectral properties of the correlators could be studied. We will leave this study for a future investigation.

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