The Proton Isovector Scalar Charge

A Lattice QCD Computation with Domain-Wall Fermions

Brandon McKinzie[1] and Meifeng Lin[2]

[1]*UC Berkeley, Berkeley, CA 94720*
[2]*Brookhaven National Laboratory, Upton, NY 11973*

Abstract

We present lattice-QCD results on the proton isovector scalar charge (g_s). The calculation is carried out with the gauge configurations generated with domain-wall fermions and Iwasaki gauge actions at $\beta = 1.75$, corresponding to a lattice cutoff scale of $a^{-1} = 1.378(7)$ GeV. We calculate g_s for two ensembles of (degenerate) light quark masses of 0.0042 and 0.001, both with momentum transfer $q^2 = 0$. An extrapolation is then made down to the physical quark mass to obtain physical value of g_s. The value of g_s describes the strength of certain short-distance interactions thought to occur in, for example, neutron decays. Further study of the isovector scalar charge is important for improving our understanding of nucleon substructure and physics beyond the Standard Model such as dark matter and supersymmetry.

I. Introduction

Lattice QCD (LQCD) is the theory of strong interactions at low momentum transfer, where the strong coupling "constant" $\alpha_s(Q^2)$ is of order unity. If we denote the Q^2 scale where the effective coupling becomes large as Λ^2, we have [1]

$$\alpha_s(Q^2) = \frac{12\pi}{(33 - 2n_f)log(Q^2/\Lambda^2)} \tag{1}$$

where n_f is the number of quark flfavors.

Therefore, as Q^2 approaches the order of Λ^2 (a typical hadronic mass), α_s becomes too large for standard perturbative methods. In this regime, a nonperturbative approach like LQCD is needed. The foundation of LQCD begins with the partition function in Euclidean space-time [2]

$$Z = \int \mathcal{D}\mathcal{A}_\mu \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S} \tag{2a}$$

$$S = \int \mathrm{d}^4x (\frac{1}{4} F_{\mu\nu}F^{\mu\nu} - \bar{\psi} M \psi) \tag{2b}$$

where S is the QCD action, $F^{\mu\nu}$ describes the gluons, ψ and $\bar{\psi}$ describe the fermions, and M is the Dirac operator. The fermions can be integrated out and S rewritten to obtain the simplified equations

$$Z = \int \mathcal{D}\mathcal{A}_\mu e^{-S} \tag{3a}$$

$$S = \int \mathrm{d}^4x (\frac{1}{4} F_{\mu\nu}F^{\mu\nu}) - \sum_i \log(\mathrm{Det}M_i) \tag{3b}$$

where the sum is over the quark flavors, distinguished by the value of the bare quark mass. Physical observables are calculated in the form of expectation values

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\mathcal{A}_\mu \mathcal{O} e^{-S} \tag{4}$$

which can be interpreted as a weighted average of $\mathcal{O}$ over all paths, with weight e^{-S}. Here $\mathcal{O}$ takes the form of time-ordered products of gauge and/or quark fields. Since the path integral is over *all* possible intermediate gauge field configurations, it is impossible to evaluate exactly. Instead, we employ a Monte Carlo (MC) procedure to perform computations, outlined as follows [3].

First, we generate a large number N_{conf} of random gauge configurations

$$A_\mu^{(\alpha)} \equiv \{A_{\mu(0)}^{(\alpha)} A_{\mu(1)}^{(\alpha)} \dots A_{\mu(N-1)}^{(\alpha)}\} \; \alpha = 1, 2, \dots, N_{conf} \tag{5}$$

where each $A_\mu^{(\alpha)}$ is a gauge field configuration on a four-dimensional space-time lattice. The configurations are sampled such that the probability $P[A_\mu^\alpha]$ for obtaining any given configuration $A_\mu^{(\alpha)}$ is

$$P[A_\mu^{(\alpha)})] \propto e^{-S[A_\mu^{(\alpha)})]} \tag{6}$$

which we identified earlier as the weight in the weighted average of (4). A possible MC estimator for $\langle \mathcal{O} \rangle$ on the discretized lattice is the straight average over the sampled configurations

$$\langle \mathcal{O} \rangle \approx \bar{\mathcal{O}} \equiv \frac{1}{N_{conf}} \sum_{\alpha=1}^{N_{conf}} \mathcal{O}[A_\mu^{(\alpha)}] \tag{7}$$

which approaches the exact value of $\langle \mathcal{O} \rangle$ as $N_{conf} \to \infty$. As will be discussed in Section II, we use the jackknife method to obtain an improved version of this estimator.

A subtle observation with profound implications in LQCD is the realization that derivatives found in $S[A_\mu^{(\alpha)}]$ are no longer continuous (on the discretized lattice). Furthermore, the term in the QCD action describing the fermions ψ discretizes differently than the term describing the gauge fields $F^{\mu\nu}$. A large part of LQCD is deciding which action discretization scheme to employ for a given analysis. In this paper, for the fermion action, we use the new Domain-Wall Fermion (DWF) discretization scheme which exhibits good chiral symmetry. The DWF action, a five-dimensional extension of the Wilson Fermion action, is [4]

$$S_{DWF} = -\sum_{x,x\prime} \sum_{s,s\prime} \bar{\psi}(x,s))[\delta_{s,s\prime} D^{\parallel}_{x,x\prime} + \delta_{x,x\prime} D^{\perp}_{s,s\prime}] \tag{8}$$

where $x, x\prime$ are four-dimensional Euclidean space-time coordinates, $s, s\prime$ are coordinates in the extra dimension (labeled from 0 to L_s-1), $D^{\parallel}_{x,x\prime}$ is the four-dimensional Wilson-Dirac operator with a mass term, and $D^{\perp}_{s,s\prime}$ is the five-dimensional analogue of the Wilson hopping term [1].

We also use the Iwasaki + DSDR gauge actions with gauge coupling $\beta = 1.75$. The lattice size is fixed at $32^3 \times 64$ with a lattice cutoff scale of $a^{-1} = 1.37$ GeV.

The quark propagators, which represent the amplitude for a quark propagating on the lattice, are found as elements of the inverse Dirac operator matrix,

$$S_F(y,j,b;x,i,a) = (M^{-1}1)^{y,j,b}_{x,i,a} \tag{9}$$

which gives the amplitude for the propagation of a quark from site x with spin-color i, a to site-spin-color y, j, b [2]. Quark propagators are typically expressed as vacuum expectation values (VEV), so-called because the quarks and inserted operators are acting to disturb the QCD vacuum. This paper is concerned with two VEV's in the form of correlation functions, denoted here by $C_{2pt}(t, \vec{P})$ and $C^{\mathcal{O}}_{3pt}(\tau, T; \vec{P})$, defined as

$$C_{2pt}(t, \vec{P}) = \left\langle N(\vec{p} = \vec{P}, t) \bar{N}(\vec{x} = 0, 0) \right\rangle \tag{10}$$

$$C^{\mathcal{O}}_{3pt}(\tau, T; \vec{P}) = \left\langle N(\vec{p} = \vec{P}, T) \mathcal{O}(\vec{p} = 0, \tau) \bar{N}(\vec{x} = 0, 0) \right\rangle \tag{11}$$

where we will take N to be the lattice proton interpolating operator. Correlation functions like these can be visualized as shown in figure 1.

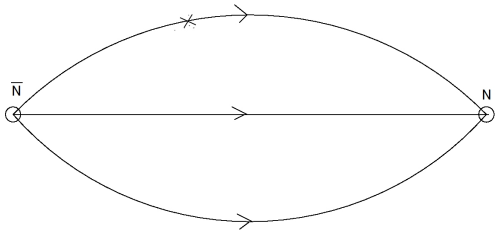

Figure 1: A correlation function diagram. From left to right, the nucleon interpolating operator creates a nucleon, operator insertions occur at intermediate X's, and the diagram ends with a nucleon annihilation operator.

Since we take up and down quarks as degenerate, there is no contribution from disconnected-loop diagrams[2]. If the insertion of $\mathcal{O}$ is sufficiently far away from both N operators in time (i.e. large τ and $T - \tau$), then contributions from excited states are negligible [5]. Taking their ratio and using this approximation yields the matrix element

$$R^{\mathcal{O}}(\tau, T; \vec{P}) = \frac{C^{\mathcal{O}}_{3pt}(\tau, T; \vec{P})}{C_{2pt}(T, \vec{P})} = \left\langle N(\vec{P}) \right| \mathcal{O} \left| N(\vec{P}) \right\rangle \tag{12}$$

Therefore, a common way of computing matrix elements in the form of (12) at fixed T is to calculate their value at different timeslices t and perform a horizontal-line fit in the so-called "plateau region". The value of the matrix element will plateau in timeslice regions with minimal excited-state contributions. We fit the data here to satisfy the approximation needed to write R in the final form of (12).

The isovector scalar charge g_s, defined in

$$\left\langle N(\vec{P}) \right| \bar{u}u - \bar{d}d \left| N(\vec{P}) \right\rangle = g_s \bar{u}(\vec{P}) u(\vec{P}) \tag{13}$$

can be computed with the aforementioned ratio-plateau method. This paper presents the computation of g_s at two different unphysical quark masses.

[1] Full definitions of these operators can be found in ref. [4] page 3. The DWF action is simply stated here to provide the reader with a visual understanding of the discretization process.

[2] Note that this statement is only true because we are working with isovector quantities.

Chiral perturbation theory (ChPT) provides the analytical prediction of how quantities like g_s should vary with the pion mass, so a chiral extrapolation can be made down to the physical quark mass to predict the true vale of g_s. The statistical methods and computational procedures used thereafter are described in Section II and Section III, respectively.

II. Jackknife Statistics and All-Mode Averaging

The Jackknife procedure, developed to correct for bias, is well-suited for calculations involving correlated samples [6]. To illustrate the technique, we let $\{\mathcal{O}\}$ denote some set containing n sampled values of an observable $\mathcal{O}$. Then, we construct a jackknife set of size n from the original sample, where the ith element is an ensemble average over all except the ith (original) element.

$$\mathcal{O}_i^{(jack)} = \frac{1}{n-1}\sum_{j\neq i}^{n}(\mathcal{O}_j) \tag{14}$$

We now have a set of n estimators which can be used for further computations. This procedure also results in simple error propagation. After a computation on each of the n jackknife estimators is performed, the final estimator is simply the set average $\langle\bar{\mathcal{O}}\rangle$, and the associated errors can be calculated directly as

$$SE^{(jack)} = \sqrt{\frac{n-1}{n}\sum_{i=1}^{n}(\langle\mathcal{O}\rangle_i - \langle\bar{\mathcal{O}}\rangle)^2} \tag{15}$$

To further reduce statistical errors, we implement all-mode averaging (AMA). Here this means relaxing the stopping condition of the conjugate gradient method when calculating the inverse of the Dirac operator so that all eigenmodes are taken into account [7]. This is especially helpful for calculations using low quark masses, where exceedingly high computational resources are necessary to obtain a decent signal to noise ratio [8], S/N, where

$$S/N(t) \propto \sqrt{N_{meas}}exp[-(M_N - \frac{3}{2}M_\pi)t] \tag{16}$$

In such cases, we can first obtain data for a large number of gauge configurations but low precision[3]. Then, we can obtain data for a much smaller number of gauge configurations but with high precision[4]. The utility of generating these different sets of data can be suggested by

$$\mathcal{O}_{imp} = \mathcal{O}_{exact} + \mathcal{O}_{appx} - \mathcal{O}_{appx} \tag{17}$$

which is (clearly) identical to the exact value. We can rewrite this equation to find the improved estimator $\mathcal{O}_{imp}$ averaged over the jackknife estimators as

$$\begin{aligned}\langle\mathcal{O}\rangle^{(imp)} = &\frac{1}{N_{appx}}\sum_{i=1}^{N_{appx}}(\mathcal{O}_i^{(appx)}) \\ &+ \frac{1}{N_{exact}}\sum_{i=1}^{N_{exact}}(\mathcal{O}_i^{(exact)} - \mathcal{O}_i^{(appx)})\end{aligned} \tag{18}$$

where $N_{appx} >> N_{exact}$, the brackets in $\langle\mathcal{O}\rangle^{(imp)}$ denote a full ensemble-average, and $\mathcal{O}_i^{(appx)}$ in the second summation is restricted access to only the type of gauge configurations used by $\mathcal{O}_i^{(exact)}$. This also provides a convenient way of analyzing how close the improved estimator is to the exact value. By increasing N_{exact} and observing the relative change in the value of $\langle\mathcal{O}\rangle^{(imp)}$, one can obtain an idea of the estimator's quality.

III. Computational Procedure

Data files representing different gauge configurations are organized into directories by source location. Here, source location refers to the time input for $\bar{N}$ from (10), and the source-sink separation[5] is a fixed nine lattice units. For the unphysical quark mass of 0.001, data is further organized into directories by *spatial* location (the spatial coordinates of $\bar{N}$ are all zero for the 0.0042 quark mass).

Once the data is properly stored and organized, the following steps outline the procedure to calculate g_s for the unphysical quark mass of 0.0042:

1. Extract the two desired correlation functions from (10) and organize the data by source location. Each file contains the correlation functions evaluated for 64 different values of τ, the time of operator insertion. At this stage, we have $N_{src} \times N_{conf}$ correlation functions, where N_{src} is the number of source locations and N_{conf} is the number of gauge configurations.
2. Average the extracted correlation values at a given gauge configuration over all different

[3] due to the relaxed stopping condition.

[4] The level of precision is limited only by the floating-point precision of the computer.

[5] Again, this refers to temporal separation. Henceforth, all "distances" mentioned can be assumed to be in time unless stated otherwise.

source locations. We are able to do this because of the translational invariance of the LQCD Lagrangian. Now we have N_{conf} number of correlation functions with improved statistics.

3. Generate two (independent) jackknife sets, $\{\langle C_{2pt}\rangle_i\}$ and $\{\langle C_{3pt}\rangle_i\}$, each of size N_{conf}. The set elements are the correlation functions averaged over gauge configurations with the ith configuration omitted[6].

4. Compute the ratio from (12) to obtain the new jackknife set $\{g_s^{jack}\}$. Each element of this set represents the calculated value of g_s for different values of time τ. Recall from Section II that the jackknife method correctly propagates errors when performing calculations such as element-by-element division of two jackknife sets.

5. Fit each element of $\{g_s^{jack}\}$ with a horizontal line in the plateau region. Various timeslice regions are fitted and a χ^2 value is computed to determine goodness-of-fit. The region with the lowest returned χ^2 value is designated as the "plateau region" for all future fits.

6. Average the $\{g_s^{jack}\}$ plots together, along with the fit result for each. The errors for the data points and final fit value are computed using the error formula in (15). The final fit value and its associated errors represent the best approximation of g_s for the given ensemble.

7. Repeat steps 1-6 for a different unphysical quark mass of 0.001. The only difference is that, for the 0.001 case, we use the AMA procedure to obtain $\{g_s^{jack}\}$. Again, we see the virtue of using the jackknife method from the fact that the approximated and exact estimators from step 3 can be added in the simple form of (18) with error propagation correctly handled in the background.

[6] See equation (14).

IV. Results

Unless stated otherwise, all quantities are presented in lattice units, defined as [9]

$$\hat{\psi}(x) = a^{3/2}\psi(x) \tag{19}$$
$$\hat{\bar{\psi}}(x) = a^{3/2}\bar{\psi}(x) \tag{20}$$
$$\hat{m}_f = am_f \tag{21}$$
$$\hat{x} = x/a \tag{22}$$

where here, $a \approx 0.144$ fm. The first primary results are the fitted values for g_s at two different unphysical quark masses of 0.0042 and 0.001, shown in figures 2 and 3, respectively. Although the AMA procedure, applied to the figure 3 data, significantly reduced the statistical error, the low signal-to-noise ratio associated with the low 0.001 quark mass (see 18) prevented the error bars from approaching the quality of figure 2. Nonetheless, there is still good agreement between the two fitted values.

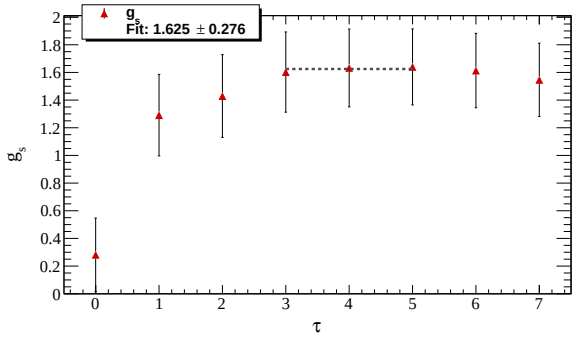

Figure 2: Unrenormalized g_s as a function of the operator insertion time τ for an unphysical quark mass of 0.0042.

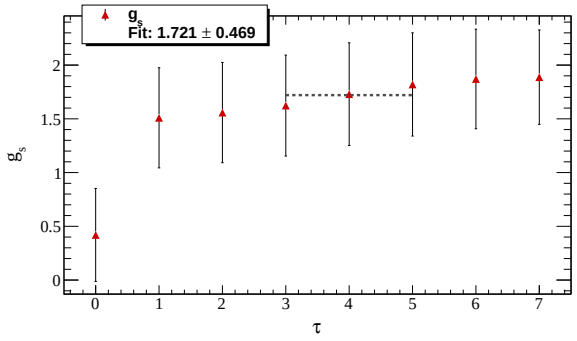

Figure 3: Unrenormalized g_s as a function of the operator insertion time τ for an unphysical quark mass of 0.001

Table 1: Conversions from the bare quark mass to the pion mass.

m_q [Lattice Units]	m_π [GeV]
0.001	0.1723
0.0042	0.2494

Before we perform the chiral extrapolation, we must renormalize g_s and convert the lattice-unit quark massess to the corresponding physical-unit pion masses. We use the renormalization factor $Z_s = 1/1.4(1)$ at the renormalization scale of 3 GeV from reference [5]. This factor is an approximation based on the spread of the calculated values for Z_m, and the error, generated to cover the spread, may be overestimated. If we denote our previous fitted result for g_s as $g_s^{(bare)}$, then

$$g_s^{(renorm)} = Z_s \times g_s^{(bare)} \tag{23}$$

$$\sigma_{g_s^{(renorm)}} = \sqrt{(g_s^{(bare)})^2(\sigma_{Z_s})^2 + (Z_s)^2(\sigma_{g_s})^2} \tag{24}$$

where $\sigma_{g_s^{(renorm)}}$ is the error of $g_s^{(renorm)}$. Next we convert each bare quark mass to the corresponding pion mass. The detailed calculations of this step can be found in table four of reference [10], but we simply quote the result in table 1 above.

Since we are working in the degenerate up and down quark limit, we will compare these values with a physical pion mass of 0.135 GeV. The renormalized values of g_s are plotted as a function of the corresponding squared pion mass in figure 4. As an approximation to ChPT, we fit these data points with a straight-line fit. With only two data points available, this is also the only sensible fitting method.

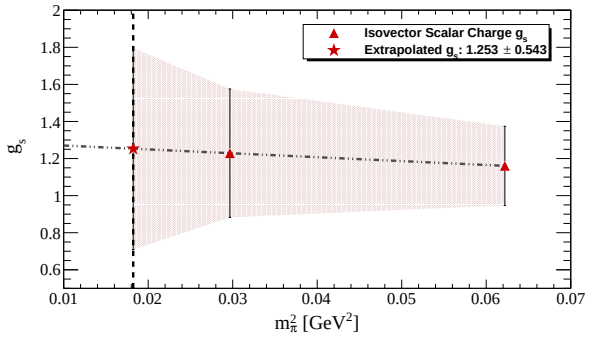

Figure 4: g_s as a function of pion mass. The line through the middle is the extrapolation of g_s to the physical pion mass (starred). The shaded region represents the approximate error of g_s in the region.

Table 2: Renormalized g_s for different pion masses. The last row contains the extrapolated result.

m_π^2 [GeV^2]	g_s
0.0297	1.229 ± 0.346
0.0622	1.161 ± 0.214
0.0182	$\mathbf{1.253 \pm 0.543}$

To obtain a true extrapolation, such as that found in figure 3 of [5], we would need more simulated data at different quark masses. We see in table 2 that g_s does not appear to vary much for different values of the quark mass.

V. Summary and Conclusions

This research offers the value of the isovector scalar charge g_s using the new domain-wall fermion discretization scheme and low quark masses. The value of g_s was calculated for two different unphysical quark masses of 0.0042 and 0.001. The fitted values for these masses were extrapolated down to the physical quark mass to obtain the best approximation for the physical g_s at 1.253 ± 0.543. Such computations are essential for understanding experimental measurements of scalar interactions in, for example, neutron beta decay. The interaction is expected to be small compared to the well-known $V - A$ structure of weak interactions, and thus few experiments have been able to measure g_s. However, new high-precision instruments are expected to be able to probe the scales necessary to measure the scalar contribution. Such measurements need precise theoretical constraints in order to convey meaningful information in a physics analysis. The results presented here both provide new constraints and strengthen former calculations of the isovector scalar charge.

VI. Acknowledgments

This project was supported in part by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI).

References

[1] F. Halzen and A. Martin, "Running Coupling Constant for QCD." *Quarks and Leptons: An Introductory Course in Modern Particle Physics.* John Wiley & Sons, 1984. 169-171. Print.

[2] R. Gupta, "Introduction to Lattice QCD", *Elsevier Science B.V.* (2008). arXiv:hep-lat/9807028.

[3] G. Lepage, "Lattice QCD for Novices", (2005). arXiv:hep-lat/0506036.

[4] S. Sasaki, T. Blum, and S. Ohta, "Lattice study of the nucleon excited states with domain wall fermions", *Phys. Rev. D* **65**, 074503 (2002).

[5] J.R. Green et al., "Nucleon Scalar and Tensor Charges from Lattice QCD with Light Wilson Quarks", *Phys. Rev. D* **86**, 114509 (2012).

[6] B. Efron, "Bootstrap Methods: Another Look at the Jackknife", *The Annals of Statistics*

[7] E. Shintani et al., "Covariant Approximation Averaging", *Phys. Rev. D* **91**, 114511 (2015).

[8] M. Lin, "Nucleon Form Factors with 2+1 Flavors of Domain Wall Fermions and All-Mode-Averaging", *Proceedings of Science* (2014). arXiv:1401.1476v1 [hep-lat] 7 Jan 2014.

[9] M. Lin. *Hadron Physics with 2+1 Flavors of Domain Wall Fermions on the Lattice*. Dissertation, Columbia University. 2007.

[10] R. Arthur et al., "Domain wall QCD with near-physical pions", *Phys. Rev. D* **87**, 094514 (2013).