Studies in hadron structure using lattice QCD with quark masses that almost reach the physical point

by

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Submitted to the Department of Physics in partial fulfillment of the requirements for the degree of

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Abstract

Lattice QCD allows us to study the structure of hadrons from first-principles calculations of quantum chromodynamics. We present calculations that shed light on the behavior of quarks inside hadrons in both qualitative and quantitative ways.

The first is a study of diquarks. We bind two quarks in a baryon with a static quark and compute the simultaneous two-quark density, including corrections for periodic boundary conditions. Defining a correlation function to isolate the intrinsic correlations of the diquark, we find that away from the immediate vicinity of the static quark, the diquark has a consistent shape, with much stronger correlations seen in the scalar diquark than in the axial-vector diquark. We present results at pion masses 293 and 940 MeV and discuss the dependence on the pion mass.

The second set of calculations is a more quantitative study that covers a wide range of (mainly isovector) nucleon observables, including the Dirac and Pauli radii, the magnetic moment, the axial charge, and the average quark momentum fraction. Two major advances over previous calculations are the use of a near-physical pion mass, which nearly eliminates the uncertainty associated with extrapolation to the physical point, and the control over systematic errors caused by excited states, which is a significant focus of this thesis. Using pion masses as low as 149 MeV and spatial box sizes as large as 5.6 fm, we show the importance of good control over excited states for obtaining successful postdictions—which we achieve for several quantities—and we identify a remaining source of systematic error that is likely responsible for disagreement with experiment in the axial sector. We then use this understanding of systematics to make predictions for observables that have not been measured experimentally.

Thesis Supervisor: John W. Negele
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Chapter 1

Introduction

The fundamental theory of the strong interaction that governs the protons and neutrons (nucleons) found inside atomic nuclei is quantum chromodynamics (QCD), which forms part of the Standard Model of particle physics. The basic ingredients of QCD are an SU(3) gauge field and a set of massive fermion fields that transform under the fundamental representation of the gauge group. When nucleons are probed at high energy, the particles associated with these fields are revealed: gluons and quarks, respectively. This occurs because QCD features asymptotic freedom, meaning that at higher energies the coupling strength becomes weaker and perturbation theory is applicable. At low energies, QCD is strongly interacting and has the property of confinement, meaning that quarks and gluons always exist in bound states (hadrons) that are singlets under the gauge group.

The only known method of doing calculations in low-energy QCD that has fully-controllable errors is lattice QCD. This is a way of regularizing QCD that preserves gauge symmetry and makes the Feynman path integral finite-dimensional and tractable using Monte Carlo methods with modern high-performance computing facilities. Lattice QCD discretizes Euclidean space-time into a four-dimensional hypercubic grid with spacing $a$, typically in a periodic box of size $L_s^3 \times L_t$, such that the vertices of the grid are located at $\mathbf{x} = a\mathbf{n}$, where $n_\mu \in \mathbb{Z}$, $0 \leq n_i \leq L_s/a$, and $0 \leq n_4 \leq L_t/a$. The quark fields $q(\mathbf{x})$ are restricted to being located on the vertices, and the gauge fields are represented by links $U_\mu(\mathbf{x})$, which are SU(3) matrices located on the edges of the grid to provide the gauge connection between adjacent vertices at $\mathbf{x}$ and $\mathbf{x} + a\hat{\mu}$.

Lattice QCD actions have the form $S_{\text{LQCD}}[U, \bar{q}, q] = S_g[U] + \bar{q}D[U]q$; in practice, the path integral for the Grassmannian quark fields is done analytically and the remaining integral over configurations of gauge links is done using importance sampling from the resulting probability distribution $p[U] \propto e^{-S_g[U]} \det D[U]$, producing an ensemble of gauge configurations. The finite lattice spacing and finite volume introduce UV and IR cutoffs; controlling errors requires removing the cutoffs using a series of ensembles that approach the continuum and infinite-volume limits. To date, this has been achieved for only a handful of observables. Furthermore, almost all calculations use larger-than-physical light quark masses (in practice, these are characterized by the pion mass), since this is less computationally expensive, and thus they also require an extrapolation to the physical pion mass.
In addition to calculations that are directly relevant to experiment, lattice QCD also provides the opportunity to study qualitative aspects of QCD that are difficult or impossible to access with experiments. Chapter 2 reports a study of this kind, looking at spatial correlations between the densities of two quarks in a baryon. In addition to helping to understand the internal structure of hadrons, the results are also relevant for judging how realistic models are that treat diquarks as pointlike degrees of freedom.

The rest of this thesis is focussed on more quantitative observables, including many that are directly probed by experiments or are relevant for analyzing results from experiments. These observables are described in Chapter 3, which concludes with a description of lattice QCD methodology and an overview of recent calculations using lattice QCD. Chapter 4 is dedicated to the study of one kind of systematic error: contributions from unwanted excited states that contaminate calculations of nucleon observables. Finally, the main quantitative results are presented in Chapter 5, which describes results from a set of calculations that includes an ensemble with a large volume and a near-physical pion mass.
Chapter 2

Spatial diquark correlations in a hadron

The notion of a diquark is used to describe the collective behavior of a pair of quarks; it have been invoked to explain many phenomena of strong interactions [APE+93]. By introducing diquarks as effective degrees of freedom in chiral perturbation theory, they have been used to explain the enhancement of $\Delta I = \frac{1}{2}$ nonleptonic weak decays [NS91]. A simple quark-diquark model is quite successful at organizing the spectrum of excited light baryon states [SW06].

The simplest diquark operators are quark bilinears with spinor part $q^T C \Gamma q$. The lowest-energy combinations are color antitriplet, even parity [Jaf05], which are divided into two kinds: the flavor symmetric scalar diquarks ($\Gamma = \gamma_5$), and the flavor antisymmetric axial-vector diquarks ($\Gamma = \gamma_i$).

Both one-gluon exchange in a quark model [DRGG75, DJJK75] and instanton [SS98] models give a spin coupling energy proportional to $\vec{S}_i \cdot \vec{S}_j$, which puts the scalar diquark at lower energy than the axial-vector diquark. The strength of this coupling falls off with increasing quark masses. For the instanton model, the effective interaction has a flavor dependence that also favors the scalar diquark. As a result, the scalar diquark is called the “good” diquark and the axial-vector diquark is called the “bad” diquark.

2.1 Earlier studies in baryons

Since diquarks are not color singlets, studying them within the framework of lattice QCD typically requires that they be combined with a third quark to form a color singlet. Diquark attractions result in spatial correlations between the two quarks in the diquark, which can be probed by computing a wavefunction or two-quark density.

In one study [BGH+07], using gauge fixing and three quarks of equal mass, a wavefunction was computed by displacing quarks at the sink,

$$\psi(r_1, r_2) \propto \sum_{r_s} \langle u(r_s + r_1, t)d(r_s + r_2, t)s(r_s, t) \times \bar{u}(\mathbf{0}, 0)d(\mathbf{0}, 0)s(\mathbf{0}, 0) \rangle.$$ (2.1)
Then, using the more convenient coordinates

$$\bm{R} = (\bm{r}_1 + \bm{r}_2)/2 \quad \text{and} \quad \bm{r} = (\bm{r}_1 - \bm{r}_2)/2$$

(Fig. 2-1 left), the wavefunction of the good and bad diquarks was shown for different fixed $R = |\bm{R}|$ as a function of $\bm{r}$, in both Coulomb gauge and Landau gauge. In all cases, the wavefunction had a peak near $\bm{r} = 0$, but it was found to fall off more rapidly for the good diquark, consistent with the expectation that good diquarks are more tightly bound.

In general, the definition of a quark wavefunction must also specify the gauge field that is associated with each configuration of quarks. In Ref. [TN94], it was found that using Coulomb gauge provides a gluon configuration that has a greater overlap with the hadron ground state than when using a string of glue, but an even greater overlap could be obtained by finding the ground-state distribution of gluons in the presence of a configuration of static quarks. Alternatively, a gauge-invariant description of the distribution of quarks can be obtained from the density of quarks, measured by placing one or more quark vector current operators on the same time slice.

In a second study [AdFL06], spatial correlations were investigated by computing the two quark density $\rho_2(\bm{r}_u, \bm{r}_d)$ for a $(u, d)$ diquark in the background of a static quark. To isolate correlations caused by the diquark interaction, analysis was restricted to spherical shells $|\bm{r}_u| = |\bm{r}_d| = r$ (Fig. 2-1 right). For both good and bad diquarks, the density was found to be concentrated near $r_{ud} = |\bm{r}_u - \bm{r}_d| = 0$, and the effect was much stronger for the good diquark. Fitting $\rho_2$ for the good diquark to $\exp(-r_{ud}/r_0(r))$, $r_0$ reached a plateau for large $r$, giving a characteristic size $r_0 = 1.1 \pm 0.2$ fm.

### 2.2 Correlation function

In the first study, the wavefunctions of good and bad diquarks were compared for an unrestricted geometry, but they were not compared against an uncorrelated wavefunction. In fact, a totally uncorrelated wavefunction could give the appearance of a diquark. Consider $\psi(\bm{r}_1, \bm{r}_2) = \phi(\bm{r}_1)\phi(\bm{r}_2)$, with $\phi(\bm{r}) = \exp(-\alpha r^2)$. Then, since $r_1^2 + r_2^2 = 2(R^2 + r^2)$, we have

$$\psi(\bm{r}_1, \bm{r}_2) = e^{-\alpha(r_1^2 + r_2^2)} = e^{-2\alpha(R^2 + r^2)}.$$
The downsides are that this divides out the tendency to stay near the static quark and retains the property of being zero if the two light quarks are uncorrelated (i.e. if \( \rho_{12} \) increases beyond the range of interactions in the system. Deviations from zero are interpreted as evidence for interactions between particles. This correlation integrates to zero and approaches zero as the relative distance \( r_{12} = |r_1 - r_2| \) increases beyond the range of interactions in the system.

The situation considered here is not so simple. The single particle density is not uniform: it is concentrated near the static quark. \( C_0 \) will still integrate to zero and fall off at large distances, however it is also larger near the static quark and this obscures the diquark correlations.

In order to remove the effect of the static quark, we define the normalized correlation function:

\[
C(r_1, r_2) = \frac{\rho_2(r_1, r_2) - \rho_1(r_1)\rho_1(r_2)}{\rho_1(r_1)\rho_1(r_2)}. \tag{2.5}
\]

This divides out the tendency to stay near the static quark and retains the property of being zero if the two light quarks are uncorrelated (i.e. if \( \rho_2(r_1, r_2) = \rho_1(r_1)\rho_1(r_2) \)). The downsides are that \( C \) no longer integrates to zero, and it is possible for \( C(r, r) \) to increase without bound as \( |r| \to \infty \). For instance, if

\[
\rho_2(r_1, r_2) \propto e^{-\left(\frac{r_1}{\alpha}\right)^2 - \left(\frac{r_2}{\beta}\right)^2},
\]

then

\[
\rho_1(r) = \int d^3r_2 \rho_2(r, r_2) \propto e^{\frac{r^2}{\alpha^2 + \beta^2}},
\]

and the correlation function is

\[
C(r_1, r_2) = c \exp \left( \frac{\alpha^2 - \beta^2}{\alpha^2(\alpha^2 + \beta^2)} R^2 + \frac{\beta^2 - \alpha^2}{\beta^2(\alpha^2 + \beta^2)} r^2 \right) - 1.
\]
If there is a tightly bound diquark, such that $\beta^2 < \alpha^2$, then this would lead to $C$ growing exponentially with $R^2$.

### 2.3 Density in a periodic box

We assume the lattice spacing is small enough that in an infinite volume we can treat $\rho_2(r_1, r_2)$ as a function of $R = |R|$, $r = |r|$, and $\theta$, the angle between $R$ and $r$. Since the calculation is actually carried out on a finite lattice volume, to recover the infinite volume result, we need to deal with the effect of periodic boundary conditions.

In a periodic box, the different possible paths of quark propagation can be divided into four classes, of which examples are shown in Figure 2-2. We are interested in the first case, which is the only surviving contribution as the box size is taken to infinity.

The problem of dealing with $\rho$ in periodic boundary conditions has been previously analyzed for the case of a meson [BGN95]. It was found that $\rho_1(r) = \sum_{n \in \mathbb{Z}^3} \tilde{\rho}_1(r + nL)$, where $\tilde{\rho}_1$ differs from the infinite volume result only for $r \gtrsim L$ due to interactions with periodic images.

These periodic image contributions to $\rho$ correspond to the second class in Fig. 2-2 in which each quark’s path wraps around the three-dimensional torus a net zero times.

In the meson case, all other paths behave like the third part of Fig. 2-2. In these cases, there is a net propagation of a colored object around the spatial direction. Like a spatial Polyakov loop, these contributions are charged under the global $\mathbb{Z}_3$ symmetry of the gluonic action, and thus have a vanishing expectation value on a quenched ensemble. On a dynamical ensemble, a sea quark can pair with the valence quark; the lowest-energy state that can propagate is a pion, so this contribution falls off as $\exp(-m_\pi L)$.

For this study, we have a baryon, and there is an additional contribution not present in mesons: from “exchange diagrams” (Fig. 2-2, far right) in which the two quarks travel in opposite directions across the periodic boundary and can form a color singlet. As the lattice size grows, this becomes dominated by the propagation of the lightest meson and so falls off as $\exp(-m_\pi L)$.

For Fig. 2-2, Example quark paths for each of the four classes. Dashed lines are identified with each other to indicate periodicity of $x$. The thick line denotes the static quark and the thin lines indicate paths for the the $u$ and $d$ quarks.
Ignoring the exchange diagrams and interactions with periodic images we find

$$\rho_2(r_1, r_2) = \sum_{n_1, n_2 \in \mathbb{Z}} \rho'_2(r_1 + n_1 L, r_2 + n_2 L),$$

(2.6)

where $\rho'_2$ is the infinite volume two quark density. In order to deal with image effects, a phenomenological fit is used. Given a good functional form $f'_2(r_1, r_2)$ for $\rho'_2$ (invariant under simultaneous rotations of $r_1$ and $r_2$ as well as exchange of $r_1$ and $r_2$), the nearest images are added in:

$$f_2(r_1, r_2) = \sum_{n_1, n_2 \in (-1,0,1)} f'_2(r_1 + n_1 L, r_2 + n_2 L).$$

(2.7)

This function and its lattice integral $f_1(r) = \sum_{r_2} f_2(r, r_2)$ can be simultaneously fit to $\rho_2$ and $\rho_1$ using a nonlinear weighted least squares method. This allows the images to be subtracted off, giving $\rho'_2 \simeq \rho_2 - f_2 + f'_2$ and $\rho'_1 \simeq \rho_1 - f_1 + f'_1$, where $f'_1(r) = \int d^3r_2 f'_2(r, r_2)$.

The static potential for interacting quarks [AdFJ03] [TSNM02] is useful for motivating the functional form. There are two main ansätze for the baryon potential, the $\Upsilon$ and $\Delta$, corresponding to flux tube shapes connecting three quarks. Both contain a sum of two-quark Coulombic potentials and a linear potential. For the $\Delta$, the linear potential grows with $r_\Delta$, the sum of two-quark distances, whereas the $\Upsilon$ case has a three-body potential that grows linearly with $r_\Upsilon$, the minimum length of a $\Upsilon$-shaped flux tube configuration joining the three quarks. Although the $\Upsilon$ potential provides the best overall fit to lattice data [TSNM02], the $\Delta$ potential works better up to distances of about 0.8 fm [dFJ05]. The $\Delta$ ansatz has also been found to better fit the nucleon wave function on the lattice [AdF02]. The $\Upsilon$ and $\Delta$ potentials differ by not more than about 15%, and here the variable $r_\Upsilon$ was not used in motivating the functional form. For a two body non-relativistic system, solutions to the Schrodinger equation with potential $1/r^2$ have the form $\exp(-r)$ near the origin. Likewise, a linear potential leads to solutions with $\exp(-r^{3/2})$ behavior at long distances. We ultimately found that the following eleven parameter functional form gave a reasonably good fit:

$$f'_2(r_1, r_2) = Ag(r_1, B, a_1, 0) g(r_2, B, a_1, 0) g(r, C, a_2, b_2)$$

$$\times \exp \left[ -D \left( r_1^{3/2} + r_2^{3/2} \right) + Er^{3/2} + Fr^{3/2} + Ge^{-\alpha \sqrt{r_1^2 + r_2^2}} \right],$$

(2.8)

with

$$g(r, A, a, b) = \begin{cases} 
\exp(-Ar) & r > a \\
 c_1 - br - c_2 r^2 & r < a 
\end{cases},$$

where $c_1, c_2$ are given by the requirement that $g$ and $\frac{\partial g}{\partial r}$ are continuous at $r = a$. The parameters are $A, \ldots, G, a_1, a_2, b_2, \text{and } \alpha$. 

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2.4 Lattice calculations

We used a mixed action scheme with domain wall valence quarks, with \( m_\pi = 293(1) \) MeV and lattice spacing \( a = 0.1241(25) \) fm. The 453 gauge configurations were generated by the MILC collaboration with asqtad staggered sea quarks, then HYP smeared (this is a gauge-covariant procedure for averaging over nearby link paths). Propagators were computed every 8 lattice units in the time direction, allowing for 8 measurements per gauge configuration, with source and sink separated by \( 8a \). Static quark propagators are given by Wilson lines; these were computed using gauge links that were HYP smeared a second time to reduce gauge noise, and measurements were averaged over seven positions for the static quark: \( x = 0 \) and the six nearest neighbors. Lattice sites that are equivalent under cubic symmetry were averaged. Errors were computed using the jackknife resampling method, with binning by gauge configuration, and fits were performed treating measurements at nonequivalent lattice sites as uncorrelated.

For comparison, we also used a heavy quark mass, with \( m_\pi \approx 940 \) MeV. Since the effects of dynamical sea quarks are negligible at that mass, we performed a calculation with \( \kappa = 0.153 \) Wilson fermions on 200 configurations from the OSU Q60a ensemble, which are \( 16^3 \times 32 \) with quenched \( \beta = 6.00 \) Wilson action. From the static quark potential, this has \( a/r_0 = 0.186 \). Using \( r_0 = 0.47 \) fm, the lattice spacing is \( a = 0.088 \) fm. We used a source-sink separation of 11 lattice units and averaged measurements over the two central timeslices.

We use smeared quarks in the baryon interpolating operator and a projection onto the non-relativistic components, \( (1 + \gamma^4)/2 \), in order to improve overlap with the ground state and minimize the effect of excited states. For the light quark ensemble, we made use of some quark propagators previously computed, and so we used the same smearing as in Ref. For the heavy quark ensemble, the source and sink were Wuppertal smeared (\( \alpha = 3.0; N = 65 \) for the good diquark, \( N = 51 \) for the bad diquark; this is defined at the start of Chapter 4) using spatially APE smeared gauge links. These parameters were chosen by tuning the number of Wuppertal smearing steps such that \( \rho_1 \) is independent of the source-sink separation; see Figs. 2-3 and 2-4.

The functions \( f_{1,2} \) were fit to a restricted set of the lattice measurements \( \rho_{1,2} \). Three conditions were imposed to reduce the influence of the points most affected by images: \( r < 8a \) for \( \rho_1 \), \( r_1^2 + r_2^2 < 100a^2 \) for \( \rho_2 \), and in both cases \( r_{\text{image}} \geq 11a \), where \( r_{\text{image}} \) is the distance to the nearest periodic image of the static quark. Fits had \( \chi^2 \) per degree of freedom ranging from 0.25 to 1.85.

In the quenched good diquark case, Figure 2-5 shows the effect of image corrections for \( \rho_1 \), and here this procedure is quite successful, even extrapolating beyond the range included in the fit.

For \( \rho_2 \), the fit works well although it is not as good as for \( \rho_1 \). Figures 2-6 and 2-7 show \( \rho_2 \) with and without image corrections. The figure on the right looks cleaner for two reasons. First, the fit function is determined using a global fit, which allows for small deviations in the points included in the plot from the specified \( R \) and \( \theta \) to be compensated for. Second, image corrections have been applied, which are substantial.
Figure 2-3: Ratio of $\rho_1$ measured at source-sink separation of 11 to $\rho_1$ at source-sink separation of 9, for the good diquark and two different smearings ($N = 65$ is displaced horizontally).

Figure 2-4: Ratio of $\rho_1(\mathbf{r})$ measured at source-sink separation of 11 to $\rho_1(\mathbf{r})$ at source-sink separation of 9, for the bad diquark and two different smearings ($N = 65$ is displaced horizontally).
2.5 Results and discussion

As a check of how well the correlation function isolates the diquark from the effect of the static quark, it is useful to compare different directions for \( r \). As Figure 2-8 shows, even at \( R = 0.2 \) fm, \( C(\mathbf{r}_1, \mathbf{r}_1) \) is independent of the direction of \( r \). The fact that at \( r = 0.2 \) fm with \( r \parallel R \), where one of the light quarks is located at the static quark,
there is no sign of the presence of the static quark, indicates that this correlation function works quite well. On the other hand, for $\rho_2$, the $R/a = 4$ data of figures 2-6 and 2-7 show a slope that changes at $r/a = 4$ for $r \parallel R$ but not for $r \perp R$.

Finally, we can compare the four cases. First, a plot of $\rho_1$ (Fig. 2-9) shows that the heavier quenched diquarks stay closer to the static quark. The difference between good and bad diquarks is much smaller, but the quenched bad and unquenched good diquarks are slightly more tightly held by the static quark.

Fig. 2-10 shows the profile of the correlation function at two fixed distances $R$ from the static quark to the center of the diquark. The good diquark has a large positive correlation at small $r$ that becomes negative at large $r$. The bad diquark has similar behavior with smaller magnitude. The difference between the good and bad diquarks is larger for the lighter pion mass, as expected from the quark mass dependence of the spin coupling that splits good and bad diquarks. As $R$ increases, both the correlation and the size of the positive region grow, although it is possible that some of this growth of $C(r_1, r_2)$ as $R$ increases may arise from the normalization of the correlation function.

At $R = 0.4$ fm, the fit agrees well with the data, and it is illustrative to look at the smooth correlation function derived from the fit. Figure 2-11 shows the full dependence of the correlation on the two independent degrees of freedom of $r$, at fixed $R = 0.4$ fm.

Our main conclusions are seen clearly in Fig. 2-11. The diquark correlations are highly independent of $\theta$, indicating negligible polarization by the heavy quark, are much stronger in the good rather than the bad channel, and increase strongly with decreasing quark mass. Finally, it is important to note that the diquark radius is approximately 0.3 fm and the hadron half-density radius is also roughly 0.3 fm, so the diquark size is comparable to the hadron size. This is reminiscent of the size of Cooper pairs in nuclei, and argues against hadron models requiring point-like diquarks.
Figure 2-8: Comparison of $\mathbf{r} \perp \mathbf{R}$ and $\mathbf{r} \parallel \mathbf{R}$ for $C(\mathbf{r}_1, \mathbf{r}_2)$ (shifted vertically), as a function of $r$ (in fm) with $R = 0.2$ fm, shown for (top to bottom) the $m_\pi = 940$ MeV and $m_\pi = 293$ MeV bad diquark, and the $m_\pi = 940$ MeV and $m_\pi = 293$ MeV good diquark.

Figure 2-9: $r^2 \rho_1(\mathbf{r})$ (in fm$^{-1}$) versus $r$ (in fm) for the good and bad diquarks on the quenched ensemble and on the dynamical ensemble.
Figure 2-10: $C(r_1, r_2)$, as a function of $r$ (in fm) with $R = 0.2$ fm (left) and $R = 0.4$ fm (right), with $r \perp R$ for the good and bad diquarks and the two pion masses.

Figure 2-11: Continuous $C(r_1, r_2)$ derived from the fit, as a function of $r$ (in fm) with $R = 0.4$ fm. The two axes $r_\parallel$ and $r_\perp$ indicate directions of $r$ parallel to and orthogonal to $R$, respectively. The color of the surface is discontinuous at $C = 0$. 

good $m_\pi = 940$ MeV

bad $m_\pi = 940$ MeV

good $m_\pi = 293$ MeV

bad $m_\pi = 293$ MeV
Chapter 3

Nucleon structure observables

The remainder of this thesis is about calculations of quantitative observables in nucleons. This chapter describes the observables in which we are interested, briefly discusses the methodology of their calculation using lattice QCD, and provides an overview of recent calculations.

3.1 Generalized parton distributions

Most of the nucleon observables that we are interested in are contained within the nucleon generalized parton distributions (GPDs) [Die03]. These parameterize matrix elements between proton states,

\[
\langle p', \lambda' | \mathcal{O}_V^q(x) | p, \lambda \rangle = \bar{u}(p', \lambda') \left( \gamma^\mu n_\mu H^q(x, \xi, t) + \frac{i n_\mu \Delta_\nu \sigma^{\mu\nu}}{2m} E^q(x, \xi, t) \right) u(p, \lambda)
\]

(3.1)

\[
\langle p', \lambda' | \mathcal{O}_A^q(x) | p, \lambda \rangle = \bar{u}(p', \lambda') \left( \gamma^\mu n_\mu \gamma_5 \tilde{H}^q(x, \xi, t) + \frac{n_\mu \Delta_\mu \gamma_5}{2m} \tilde{E}^q(x, \xi, t) \right) u(p, \lambda),
\]

(3.2)

where \( \Delta = p' - p, t = -\Delta^2, \xi = -\frac{n_\mu \Delta_\mu}{2}, n_\mu \) is a lightcone vector, and

\[
\mathcal{O}_V^q(x) = \int \frac{d\lambda}{4\pi} e^{i \lambda x} \bar{q}(\frac{\lambda n_2}{2}) \gamma^\mu n_\mu U(\frac{\lambda n_2}{2}, \frac{\lambda n_2}{2}) q(\frac{\lambda n_2}{2})
\]

(3.3)

\[
\mathcal{O}_A^q(x) = \int \frac{d\lambda}{4\pi} e^{i \lambda x} \bar{q}(\frac{\lambda n_2}{2}) \gamma^\mu n_\mu \gamma_5 U(\frac{\lambda n_2}{2}, \frac{\lambda n_2}{2}) q(\frac{\lambda n_2}{2})
\]

(3.4)

are bilocal operators with \( U(x, y) \) a Wilson line. The parameter \( x \) corresponds to the fraction of longitudinal momentum carried by the quark \( q \).

These GPDs contain, in the infinite momentum frame, the distribution of quarks with respect to transverse position and longitudinal momentum [Bur03]. They contain both the elastic-scattering form factors (when integrated over \( x \); see the next section), and (in the forward limit) the ordinary parton distribution functions \( q(x) \) and \( \Delta q(x) \) that are probed in deep-inelastic scattering.

Convolutions of GPDs are measured in colliders via exclusive processes such as
deeply virtual Compton scattering. Lattice QCD calculations can access the generalized form factors, which provide complementary information about GPDs and are the subject of the next section.

### 3.2 Generalized form factors

Moments in $x^n$ of the GPDs give generalized form factors (GFFs),

\[
\int_{-1}^{1} dx \, x^n H^q(x, \xi, t) = \sum_{i=0, \text{even}}^{n} (2\xi)^i A_{n+1,i}^q(t) + (n \mod 2)(2\xi)^{n+1} C_{n+1}^q(t) \tag{3.5}
\]

\[
\int_{-1}^{1} dx \, x^n E^q(x, \xi, t) = \sum_{i=0, \text{even}}^{n} (2\xi)^i B_{n+1,i}^q(t) - (n \mod 2)(2\xi)^{n+1} C_{n+1}^q(t) \tag{3.6}
\]

\[
\int_{-1}^{1} dx \, x^n \tilde{H}^q(x, \xi, t) = \sum_{i=0, \text{even}}^{n} (2\xi)^i \tilde{A}_{n+1,i}^q(t) \tag{3.7}
\]

\[
\int_{-1}^{1} dx \, x^n \tilde{E}^q(x, \xi, t) = \sum_{i=0, \text{even}}^{n} (2\xi)^i \tilde{B}_{n+1,i}^q(t), \tag{3.8}
\]

and these parameterize matrix elements of twist-two operators, e.g.,

\[
\langle p', \lambda' | \bar{q} \gamma^\mu q | p, \lambda \rangle = \bar{u}(p', \lambda') \left( \gamma^\mu A_{10}^q(t) + \frac{i\sigma^{\mu\nu}\Delta_{\nu}}{2m} B_{10}^q(t) \right) u(p, \lambda) \tag{3.9}
\]

\[
\langle p', \lambda' | \bar{q} \gamma^\mu \gamma_5 q | p, \lambda \rangle = \bar{u}(p', \lambda') \left( \gamma^\mu \tilde{A}_{10}^q(t) + \frac{\Delta^\mu}{2m} \tilde{B}_{10}^q(t) \right) \gamma_5 u(p, \lambda) \tag{3.10}
\]

\[
\langle p', \lambda' | \bar{q} \gamma^\mu i \gamma_5 \vec{D}^\nu q | p, \lambda \rangle = \bar{u}(p', \lambda') \left( \bar{p}^\mu \gamma^\nu A_{20}^q(t) + \frac{i\bar{p}^\mu \sigma^{\mu\nu} \Delta_{\nu}}{2m} B_{20}^q(t) \right.
\]

\[
\left. + \frac{\Delta^\mu \Delta^\nu}{m} C_{2}^q(t) \right) u(p, \lambda), \tag{3.11}
\]

where $\bar{p} = (p + p')/2$ and the braces denote taking the symmetric traceless part.

It is easy to recognize the Dirac and Pauli form factors associated with the vector current,

\[
F_1^q(t) = A_{10}^q(t), \quad F_2^q(t) = B_{10}^q(t), \tag{3.12}
\]

as well as the axial and induced pseudoscalar form factors,

\[
G_A^q(t) = \tilde{A}_{10}^q(t), \quad G_P(t) = \tilde{B}_{10}^q(t). \tag{3.13}
\]

Because it can be computed without computationally-demanding disconnected quark contractions, we will focus on the isovector combination,

\[
F_{1,2}^v(t) = F_{1,2}^u(t) - F_{1,2}^d(t) = F_{1,2}^p(t) - F_{1,2}^n(t), \tag{3.14}
\]
where $F_{1,2}^{p,n}(t)$ are form factors of the electromagnetic current in a proton and in a neutron, respectively. We will also consider the isoscalar combination,

$$F_{1,2}^{s}(t) = \frac{1}{3} \left( F_{1,2}^{u}(t) + F_{1,2}^{d}(t) \right) = F_{1,2}^{p}(t) + F_{1,2}^{n}(t). \quad (3.15)$$

For the other form factors, we will likewise focus on the isovector combination.

The behavior of the vector form factors near zero momentum transfer is particularly interesting:

$$F_{1}^{v}(t) = g_{V} \left( 1 - \frac{1}{6} (r_{1}^{2})^{v} t + O(t^2) \right), \quad (3.16)$$

$$F_{2}^{v}(t) = \kappa^{v} \left( 1 - \frac{1}{6} (r_{2}^{2})^{v} t + O(t^2) \right), \quad (3.17)$$

where $g_{V} = 1$, $\kappa^{v} = \kappa^{p} - \kappa^{n}$ is the isovector anomalous magnetic moment, and $(r_{1}^{2})^{v} = (r_{1}^{2})^{p} - (r_{1}^{2})^{n}$ and $(r_{2}^{2})^{v} = (\kappa^{p}(r_{2}^{2})^{p} - \kappa^{n}(r_{2}^{2})^{n})/\kappa^{v}$ are the isovector Dirac and Pauli squared radii (the isoscalar radii are defined analogously). These are related to the mean-squared charge and magnetic radii:

$$(r_{1}^{2})^{p,n} = (r_{E}^{2})^{p,n} - \frac{3 \kappa^{p,n}}{2 m_{p,n}^{2}}, \quad (3.18)$$

$$(r_{2}^{2})^{p,n} = \frac{\mu^{p,n}(r_{M}^{2})^{p,n} - (r_{E}^{2})^{p,n}}{\kappa^{p,n}} + \frac{3}{2 m_{p,n}^{2}}. \quad (3.19)$$

There is a $7\sigma$ discrepancy between a recent determination of the proton charge radius $\sqrt{(r_{E}^{2})^{p}}$ from its effect on energy levels measured in muonic hydrogen [ANS+13] and the CODATA 2010 value [MTN12] based on electron-proton scattering and spectroscopy; a reliable calculation from theory may help to resolve the issue.

Near zero momentum transfer, the isovector axial form factor can be parameterized as follows:

$$G_{A}^{v}(t) = g_{A} \left( 1 - \frac{1}{6} (r_{A}^{2})^{v} t + O(t^2) \right), \quad (3.20)$$

where $g_{A}$ is the axial charge (discussed in the next section) and $(r_{A}^{2})^{v}$ is the mean-squared axial radius. The axial form factor $G_{A}$ has been measured in (quasi-)elastic neutrino scattering experiments, and serves as an input to models used for neutrino-oscillation experiments. The isovector induced pseudoscalar form factor has a pion pole that dominates the behavior near zero momentum transfer; $G_{v}^{P}$ has been measured in muon capture experiments, including a recent precise measurement of the rate of ordinary muon capture on the proton [A+13] that found $g_{P}^{*} \equiv \frac{m_{\mu}}{2 m_{N}^{2}} G_{v}^{P}(0.88 m_{\mu}^{2}) = 8.06(55)$.

The GFFs $A_{20}^{q}(t)$ and $B_{20}(t)$ give information about longitudinal momentum and angular momentum in a nucleon. The forward matrix element of the quark energy-momentum operator yields $A_{20}^{q}(0) = \langle x \rangle_{q}$, which is the average longitudinal momentum fraction carried by quarks $q$ and $\bar{q}$. In the Ji decomposition [Ji97], the total angular
momentum carried by quarks is given by \( J^q = \frac{1}{2}(A^q_{20}(0) + B^q_{20}(0)) \). Using also the quark spin contribution to the nucleon angular momentum, \( \frac{1}{2} \Delta \Sigma^q = \frac{1}{2} \tilde{A}^q_{10}(0) \), this gives the contribution from quark orbital angular momentum, \( L^q = J^q - \frac{1}{2} \Delta \Sigma^q \).

### 3.3 Neutron beta decay couplings

To first approximation, neutron beta decay depends on two neutron-to-proton transition matrix elements at zero momentum transfer:

\[
\langle p | \bar{u} \gamma^\mu d | n \rangle = g_V \bar{u}_p \gamma^\mu u_n \tag{3.21}
\]
\[
\langle p | \bar{u} \gamma^\mu \gamma_5 d | n \rangle = g_A \bar{u}_p \gamma^\mu \gamma_5 u_n, \tag{3.22}
\]

and in the isospin limit we have \( g_V = F_1^{u-d}(0) = 1 \) and \( g_A = G_A^{u-d}(0) \). Beta decay experiments have measured \( g_A/g_V = 1.2701(25) \) \[\text{[B+12]}\]. The leading corrections include recoil effects that depend on the isovector anomalous magnetic moment \( \kappa^v = F_2^{u-d}(0) \). It has been shown \[\text{[BCC+12]}\] that, if one generically assumes new (beyond the Standard Model) physics induces effective four-fermion couplings between quarks and leptons, then the resulting leading effects on neutron beta decay depend on the matrix elements of scalar and tensor bilinears,

\[
\langle p | \bar{u} d | n \rangle = g_S \bar{u}_p u_n \tag{3.23}
\]
\[
\langle p | \bar{u} \sigma^{\mu \nu} d | n \rangle = g_T \bar{u}_p \sigma^{\mu \nu} u_n. \tag{3.24}
\]

The scalar and tensor charges, \( g_S \) and \( g_T \), have not been measured experimentally, and thus they present an opportunity for lattice QCD calculations to provide useful input for determining the sensitivity of beta decay experiments to new physics.

In addition, isospin symmetry equates the scalar charge with a matrix element of \( \bar{u}u - \bar{d}d \) between proton states, and the Feynman-Hellmann theorem implies that

\[
g_S = \left( \frac{\partial}{\partial m_u} - \frac{\partial}{\partial m_d} \right) m_p, \tag{3.25}
\]

i.e., \( g_S \) controls the leading-order contribution from light quark mass splitting to the neutron-proton mass difference.

The tensor charge is also the first moment of transversity: \( g_T = \langle 1 \rangle_{\delta_u - \delta_d} \). It will be measured at Jefferson Lab using the 12 GeV upgrade \[\text{[DEE+12]}\].
3.4 Lattice QCD methodology

In order to measure nucleon matrix elements in Lattice QCD, we compute nucleon two-point and three-point functions,

\[ C_{2pt}(\vec{p}, t) = \sum_{\vec{x}} e^{-i\vec{p} \cdot \vec{x}} \text{Tr}[\Gamma_{\text{pol}}(N(\vec{x}, t)\bar{N}(0, 0))] \]  \hspace{1cm} (3.26)

\[ C_{3pt}^{\alpha\beta}(\vec{p}, \vec{p}', \tau, T) = \sum_{\vec{x}, \vec{y}} e^{-i\vec{p}' \cdot \vec{x}} e^{i(\vec{p} - \vec{p}') \cdot y} \text{Tr}[\Gamma_{\text{pol}}(N(\vec{x}, T)\mathcal{O}^q(\vec{y}, \tau)\bar{N}(0, 0))], \]  \hspace{1cm} (3.27)

where \( N \) is a proton interpolating operator, \( \mathcal{O}^q \) is the \( \bar{q} \ldots q \) operator whose matrix elements we want to compute, and \( \Gamma_{\text{pol}} = \frac{1+i\gamma_4}{2} \frac{1-i\gamma_5}{2} \) is a spin and parity projection matrix. The three-point correlators have contributions from both connected and disconnected quark contractions, but we compute only the connected part. Omitting the disconnected part (where \( \mathcal{O}^q \) is attached to a quark loop) introduces an uncontrolled systematic error except when taking the \( u - d \) (isovector) flavor combination, where the disconnected contributions cancel out.

On a lattice with finite time extent \( L_t \), the transfer matrix formalism yields

\[ C_{2pt}(\vec{p}, t) = \sum_{n,m} e^{-E_n L_t} e^{-(E_n - E_m) t} \sum_{\alpha,\beta} (\Gamma_{\text{pol}})_{\alpha\beta} \sum_{\vec{x}} e^{-i\vec{p} \cdot \vec{x}} \langle m|N_\beta(\vec{x})|n\rangle \langle n|\bar{N}_\alpha(0)|m\rangle \]  \hspace{1cm} (3.28)

\[ C_{3pt}^{\alpha\beta}(\vec{p}, \vec{p}', \tau, T) = \sum_{n,n',m} e^{-E_n L_t} e^{-(E_n - E_m) \tau} e^{-(E_{n'} - E_m)(T-\tau)} \sum_{\alpha,\beta} (\Gamma_{\text{pol}})_{\alpha\beta} \times \sum_{\vec{x},\vec{y}} e^{-i\vec{p}' \cdot \vec{x}} e^{i(\vec{p} - \vec{p}') \cdot y} \langle m|N_\beta(\vec{x})|n\rangle \langle n'|\mathcal{O}^q(\vec{y})|n\rangle \langle n|\bar{N}_\alpha(0)|m\rangle. \]  \hspace{1cm} (3.29)

Thermal contamination is eliminated in the large \( L_t \) (zero-temperature) limit, in which state \( m \) is the vacuum, and states \( n \) and \( n' \) are restricted to having the quantum numbers of a proton with momentum \( \vec{p} \) and \( \vec{p}' \), respectively. Unwanted contributions from excited states can be eliminated by then taking \( \tau \) and \( T - \tau \) to be large. Matrix elements are computed from an appropriate ratio of \( C_{3pt} \) and \( C_{2pt} \), or other methods; this is discussed in more detail in Section 4.2.

In order to compute \( C_{3pt} \), we use sequential propagators through the sink. This has the advantage of allowing for any operator to be measured at any time using a fixed set of quark propagators, but new backward propagators must be computed for each source-sink separation \( T \). Increasing \( T \) suppresses excited-state contamination, but it also increases the noise; the signal-to-noise ratio is expected to decay asymptotically as \( e^{-(m_N - \frac{1}{2}m_r)T} \) \[\text{Lep89}\]. Past calculations have often used a single source-sink separation, which only allows for a limited ability to identify and remove excited state contamination. In particular, when computing forward matrix elements, there is no way of distinguishing contributions from excited states with \( n' = n \) from the ground state contribution, when using \( C_{3pt} \) with a single \( T \).

To compute form factors: for each value of \( Q^2 = -(p' - p)^2 \), we parameterize
the corresponding set of matrix elements of \( O \) by form factors (e.g., \( F_1^q(Q^2) \) and \( F_2^q(Q^2) \)), and perform a linear fit to solve the resulting overdetermined system of equations, after first combining equivalent matrix elements to improve the condition number \[ SBL^{+10} \]. This approach makes use of all available matrix elements in order to minimize the statistical error in the resulting form factors.

### 3.5 Past calculations

For several years, elastic and generalized nucleon form factors have been computed using lattice QCD; see Tab. 3.1 for a summary of calculations done in recent years. To reduce the computational cost, past calculations have used quark masses somewhat larger than the physical quark masses, corresponding to a pion mass twice the physical value or more. Where comparison with experiment is possible, calculations done using heavier-than-physical quarks often disagreed with experiment. For instance, it is common for the computed isovector Dirac radius \( (r^2)^v \) to be roughly half of the experimental value and for the isovector quark momentum fraction \( \langle x \rangle_{u-d} \) to be about 50% larger than the phenomenological result. In order to compare with experiment, past calculations have relied heavily on extrapolation to the physical pion mass using chiral perturbation theory (ChPT), which allows for rapid variation as \( m_\pi \) approaches zero. Since it is unclear how large the range of pion masses is over which ChPT is reliable, calculations near the physical pion mass are essential for reducing the uncertainty associated with extrapolation.

In addition to heavier-than-physical quarks, there has been much attention paid to finite-volume effects as sources of systematic error \[ YAB^{+08}, LO12, HLY13 \], but in the last few years, the problem of unwanted contributions from excited states has also seen increased attention. Ref. \[ CGH^{+11} \] included a dedicated study at \( m_\pi = 660 \text{ MeV} \) in which the source-sink separation was varied between \( T = 0.79 \) and 1.37 fm and the conclusion was that excited-state effects in \( F_1^v(Q^2) \) were negligible. The same conclusion was reached in Ref. \[ SBL^{+10} \] when comparing \( F_1^v, F_2^v(Q^2) \) at \( T = 1.01 \) and 1.18 fm using a reduced-statistics calculation at \( m_\pi = 297 \text{ MeV} \) and in Ref. \[ BEE^{+10} \] when comparing \( g_A \) at \( T = 1.12 \) and 1.24 fm using a reduced-statistics calculation at \( m_\pi = 356 \text{ MeV} \). An alternative approach for computing three-point correlators is the open sink method, where the source-operator separation \( \tau \) and the operator \( O \) are fixed, allowing for all source-sink separations to be computed at the same time. This was explored in Ref. \[ DAC^{+11} \] using \( m_\pi \approx 380 \text{ MeV} \), comparing \( g_A \) with \( \tau = 0.70 \text{ fm} \) and \( \langle x \rangle_{u-d} \) with \( \tau = 0.86 \text{ fm} \) against a fixed-sink calculation with \( T = 0.94 \text{ fm} \); the authors concluded that excited states had a negligible effect on \( g_A \) but caused \( \langle x \rangle_{u-d} \) to increase by 10%. The open sink method was also used in Ref. \[ ODK^{+13} \], where \( g_A \) was studied with \( m_\pi \approx 290 \text{ MeV} \) and \( \tau = 0.46 \text{ fm} \), using a variational basis of four nucleon interpolating operators of different spatial sizes. The authors found that if the nucleon operator was too small, the calculated value of \( g_A \) was about 10% smaller than the result obtained from using the full basis of operators.

The study of excited-state systematics is a major focus of this thesis. Other than the results presented here (some of which were previously reported in Refs. \[ GNP^{+11} \]
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</tbody>
</table>

Table 3.1: Recent lattice QCD calculations of nucleon isovector generalized form factors and the connected part of isoscalar generalization form factors. $N_{\text{f}}=2$ means degenerate $u$ and $d$ quarks, $N_{\text{f}}=2+1$ adds a dynamical $s$ quark, and $N_{\text{f}}=2+1+1$ adds a $c$ quark to the action. $N_{\text{ens}}$ is the number of lattice QCD ensembles used, $m_\pi$ is the pion mass, $L_s$ is the spatial box size, $a$ is the lattice spacing, and $T$ is the source-sink separation.

References:
- Ref. [GBJ+12] reports the pion mass on the additional ensemble as 130 MeV after correcting for finite-volume effects.
- Ref. [HNN+12] also reports calculations in progress on four additional ensembles similar to the existing two but with $a = 0.06$ and 0.09 fm.
- Only preliminary (not renormalized) results are presented.

Note: $\Delta u = \Delta d$ is the spatial box size.
the only calculations listed in Tab. 3.1 that consistently uses multiple source-sink separations on every ensemble are the in-progress calculations reported by Ref. [GBJ+12] and the calculation of $g_A$ in Ref. [CDMvH+12]. In the latter, the extrapolated value of $g_A$ at the physical pion mass only agreed with experiment when excited-state effects were well-controlled.
Chapter 4

Excited-state systematic errors

Lattice QCD calculations of nucleon matrix elements have typically used a single source-sink separation with a single nucleon interpolating operator,

$$N_\alpha(x) = \epsilon^{\alpha bc} \left( \bar{u}_\beta^a(x)(C\gamma_5)_{\beta\delta}\bar{d}_\delta^b(x) \right) \bar{u}_\alpha^c(x),$$  \hspace{1cm} (4.1)

where $\bar{q}$ is a smeared quark field. A common smearing technique is Wuppertal (gauge-covariant approximately Gaussian) smearing \[Gus90\]:

$$\tilde{q} = \left( 1 - \frac{\sigma^2 \nabla^2}{4N} \right)^N q = \left( 1 - \frac{3\sigma^2}{2N} \right)^N (1 + \alpha H)^N q,$$  \hspace{1cm} (4.2)

which is parameterized by $(\sigma, N)$ or $(\alpha, N)$, where $\alpha = \frac{\sigma^2/4N}{1-3\sigma^2/2N}$, $H$ is the spatial hopping matrix,

$$Hq(x) = \sum_{i=1}^{3} \left( \bar{U}_i(x)q(x+i) + \bar{U}_i^\dagger(x-i)q(x-i) \right),$$  \hspace{1cm} (4.3)

and $\bar{U}$ is the gauge field, usually having been smeared to reduce noise using a gauge-covariant procedure. In a typical calculation, the parameters are varied (e.g., by adjusting $N$ with fixed $\alpha$) to maximize the overlap between $N_\alpha(x)$ and the nucleon ground state; a tuned source of this type can reach roughly 50% overlap with the ground state \[DBC^+02\]. Excited states are then filtered out using their more-rapid decay with Euclidean time.

There are two natural avenues of improving on the usual situation: either using an improved interpolating operator that has a lower overlap with low-lying excited states, or making greater use of the Euclidean time separation as a means of filtering out excited-state contaminations.
4.1 Improved nucleon interpolating operators

A systematic approach for finding an interpolating operator that has reduced or zero overlap with the lowest-lying excited states is the variational method \[ LW90 \] where, given a basis of \( N \) interpolating operators \( O_i \), one finds the optimal linear combination. This involves computing the matrix of two-point correlators,\

\[ C_{ij}(t) = \langle O_i(t)O_j^\dagger(0) \rangle, \]

and solving the generalized eigenvalue problem,\

\[ C_{ij}(t) v_j(t, t_0) = \lambda(t, t_0) C_{ij}(t_0) v_j(t, t_0). \]

It has been shown \[ BDMvh09 \] that, if the reference time \( t_0 \) is varied with \( t \) such that \( t_0 \geq t/2 \), then the effective energies \( E_{\text{eff}}(t) = -\partial_t \log \lambda(t, t_0) \) will equal the energies of the lowest-lying \( N \) states, up to errors that decay asymptotically as \( e^{-(E_{N+1}-E_n)t} \). Thus the effect of the first \( N-1 \) excited states can be removed when computing the ground-state energy. A similar result was shown for using the eigenvectors \( v_i(t, t_0) \) to select linear combinations of \( O_i \) for computing three-point functions (and thus matrix elements).

4.1.1 Nucleon interpolating operators with up to two derivatives

A natural way of obtaining a larger basis of nucleon interpolating operators is to construct three-quark operators including derivatives applied to the quark fields. This allows for the quarks to have angular momentum and for correlations to exist between the quarks, which is not the case for the standard S-wave uncorrelated 3-quark operator.

The standard operator consisting of a product of three Gaussian-distributed quarks is analogous to the zeroth-order wave function in the Isgur-Karl nonrelativistic quark model \[ IK78, IK79b, IK79a \]. In this model, additional wavefunctions were constructed from the harmonic oscillator basis, and it was found that \[ IKK78 \]

\[ |N\rangle \simeq 0.90|2S_2\rangle - 0.34|2S_2'\rangle - 0.27|2S_M\rangle - 0.06|4D_M\rangle, \]

where \( |2S_{L_\Pi}\rangle \) denotes a wavefunction with spin \( S \), angular momentum \( L \). The symmetry index \( \Pi \) denotes the behavior under permutation of the spatial wavefunctions of the quarks, labelled by an irreducible representation of the permutation group \( S_3 \): symmetric \( S \), antisymmetric \( A \), or the two-dimensional mixed-symmetry irrep \( M \). The wavefunction \( 2S_S \) is the zeroth-order (Gaussian) wave function, and the others all feature two harmonic-oscillator excitations — including \( 2S_S' \), for which the prime serves to distinguish it from the zeroth-order wave function.

Applying covariant derivatives to the Gaussian-smeared quark fields can be used to create interpolating operators that are analogous to these wavefunctions with excited harmonic oscillators. In addition, because we are using relativistic quarks, there are
many more possible operators. For each operator, the quarks have spatial ($\psi$), flavor ($\chi$), internal spin ($\xi$) and parity ($\pi$), and color degrees of freedom. To form color singlets, the color part is always antisymmetric, so the remainder must be symmetric. Each degree of freedom will be classified according to its behavior under permutation of the quarks; the multiplication table of the irreps of this permutation group is given in Tab. 4.1. We also denote the two rows of the $M$ irrep as $MA$, which is antisymmetric under exchange of the first two indices, and $MS$, which is symmetric under their exchange. From this, it is clear that in the product $M \times M$, $MS \times MS$ and $MA \times MA$ contribute to $S$ and $MS$, whereas $MS \times MA$ and $MA \times MS$ contribute to $A$ and $MA$.

Beginning with flavor: there are three permutations of $uud$; these yield two different proton combinations,

$$
\chi_p^{MA} = \frac{1}{\sqrt{2}} (udu - duu) \quad \chi_p^{MS} = \frac{1}{\sqrt{6}} (udu + duu - 2uuu),
$$

as well as the symmetric $\Delta^+$ combination. In practice, we will use $udu$ as the flavor part of the operator, and arrange that the rest of the operator is symmetric under exchange of the first two indices. The fermion antisymmetry will be imposed when we compute quark contractions on the lattice, and this will project out $\chi_p^{MA}$.

For internal quark spin there are, e.g., two $S = \frac{1}{2}$, $S_z = \frac{1}{2}$ combinations,

$$
\xi^{MA}_\uparrow = \frac{1}{\sqrt{2}} (\uparrow\downarrow\uparrow - \downarrow\uparrow\uparrow) \quad \xi^{MS}_\uparrow = \frac{1}{\sqrt{6}} (\uparrow\downarrow\uparrow + \downarrow\uparrow\uparrow - 2 \uparrow\uparrow\downarrow).
$$

Regardless of $S_z$, the $\xi^{MA}$ combinations have the first two quarks in spin zero, the $\xi^{MS}$ have them in spin one with total spin $\frac{1}{2}$, and the symmetric combination $\xi^S$ has them in spin one with total spin $\frac{3}{2}$.

Unlike in the non-relativistic quark model, relativistic quarks can have both positive and negative internal parity, and these can be accessed via the parity projections $\frac{1+\gamma_4}{2}q$. This can yield, for example, overall positive internal parity from either three positive-parity quarks or one positive-parity and two negative-parity quarks:

$$
\pi_+^{S1} = (++) \quad \pi_+^{S2} = \frac{1}{\sqrt{3}} ((+-+) + (-++) + (-+-)) \\
\pi_+^{MA} = \frac{1}{\sqrt{2}} ((-+-) - (++-)) \quad \pi_+^{MS} = \frac{1}{\sqrt{6}} ((+-+) + (++-) - 2(-+-)).
$$

An equivalent set with overall negative parity can be obtained by exchanging $+$ and $-$.
Table 4.2: Quark bilinears. The index Π indicates whether the bilinear is symmetric or antisymmetric under exchange of internal spin and parity (i.e. Dirac spin) between the two quarks.

<table>
<thead>
<tr>
<th>Γ in ( u^T C T d )</th>
<th>( S^P_\Pi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \gamma_5, \gamma_5 \gamma_4 )</td>
<td>( 0^+_A )</td>
</tr>
<tr>
<td>( 1 )</td>
<td>( 0^-_A )</td>
</tr>
<tr>
<td>( \gamma_4 )</td>
<td>( 0^-_S )</td>
</tr>
<tr>
<td>( \gamma_j, \gamma_j \gamma_4 )</td>
<td>( 1^+_S )</td>
</tr>
<tr>
<td>( \gamma_j \gamma_5 )</td>
<td>( 1^-_S )</td>
</tr>
<tr>
<td>( \gamma_j \gamma_5 \gamma_4 )</td>
<td>( 1^-_S )</td>
</tr>
</tbody>
</table>

above. Operators constructed with \( \pi^{S1}_A \) use the positive-parity part of all three quarks, and are the closest analogs of the nonrelativistic quark-model wavefunctions.

Table 4.2 lists the properties of quark bilinears constructed with the standard notation of Dirac spinors and gamma matrices; this is useful for constructing the three-quark operators. For instance, if an operator has \( \xi^{MS} \pi^{MA}_+ \), then the first two quarks are spin-one and antisymmetric, which implies that they have negative parity. Overall, the three quarks will have \( S^P = \frac{1}{2} \). Remembering that we use a \( \frac{1+\gamma_4}{2} \) parity-projection in two-point and three-point correlators, we find that the corresponding three-quark operator will look like \( (u^T C \gamma_j \gamma_5 d) \gamma_j u \). The \( \gamma_j \) in front of the third quark serves to yield overall spin \( \frac{3}{2} \), and the parity-projection will project onto the negative-parity part of the third quark, so that the overall parity is positive.

For the standard operator with no derivatives, the spatial part factorizes as follows:

\[
\psi(r_1, r_2, r_3) = \phi^{(1)}(r_1) \phi^{(2)}(r_2) \phi^{(3)}(r_3). \tag{4.10}
\]

Because we don’t want to change the center-of-mass behavior, it is useful to consider the change of coordinates,

\[
\rho = \frac{1}{\sqrt{2}}(r_1 - r_2), \quad \lambda = \frac{1}{\sqrt{6}}(r_1 + r_2 - 2r_3), \quad R = \frac{1}{3}(r_1 + r_2 + r_3); \tag{4.11}
\]

we are seeking combinations of derivatives that correspond to excitations in the \( \rho \) and \( \lambda \) coordinates but not in the \( R \) coordinate. This is equivalent to avoiding total derivatives with respect to the overall position of the operator; such an operator would vanish at zero momentum in the continuum.

We will use the symbol \( \psi^\Pi_{L}^{(n_1n_2n_3)} \) to denote a spatial configuration with \( n_i \) derivatives applied to the three quark fields with permutation symmetry \( \Pi \), and angular momentum \( L \). Starting with zero derivatives, there is only \( \psi_0^{S(000)} \). For a nucleon, we always have \( \chi^M \), and to get \( J = \frac{1}{2} \) we need \( S = \frac{1}{2} \) and thus \( \xi^M \). To get an overall symmetric operator, the remaining \( \pi \) part can have either \( M \) or \( S \) symmetry. Again recognizing that we will project onto the symmetric part, we get three independent operators:

\[
^2 S_{S1,2,3} = \psi_0^{S(000)}(udu) \xi^{MA}_+ \pi^{S1,S2,MS}_+. \tag{4.12}
\]
Consulting Tab. 4.2 for the symmetry properties of quark bilinears, we see that the operator with $\pi_{S1}^+$ is the standard operator with a positive parity projection in the diquark part:

$$N(2S_{S1})_\alpha(x) = \epsilon^{abc} \left( \bar{u}^T_a(x) C \gamma_5 \frac{1+\gamma_4}{2} \tilde{d}_b(x) \right) \tilde{u}_{ca}(x),$$

(4.13)

and the other two are linear combinations of operators $(u^T C \gamma_5 \frac{1-\gamma_4}{2} d) u$ and $(u^T C d) \gamma_5 u$.

With one derivative, we have $L = 1$ and three independent spatial parts $\psi_1^{S(100)}$, $\psi_1^{MS(100)}$, and $\psi_1^{MA(100)}$, which correspond to taking derivatives in the $R$, $\lambda$, and $\rho$ coordinates, respectively. We leave out the first one; explicitly, the other two are

$$\psi_{1,i}^{MS(100)} = \frac{1}{\sqrt{6}} ( (D_i \phi^{(1)}) \phi^{(2)} \phi^{(3)} + \phi^{(1)} (D_i \phi^{(2)}) \phi^{(3)} - 2 \phi^{(1)} \phi^{(2)} (D_i \phi^{(3)}))$$

$$\psi_{1,i}^{MA(100)} = \frac{1}{\sqrt{2}} ( (D_i \phi^{(1)}) \phi^{(2)} \phi^{(3)} - \phi^{(1)} (D_i \phi^{(2)}) \phi^{(3)}).$$

(4.14)

For $J = \frac{1}{2}$, the quarks can have $S = \frac{1}{2}$ or $S = \frac{3}{2}$. Starting with the former: the spatial, flavor, and spin have mixed symmetry. Choosing the symmetric quark parity combinations yields two operators,

$$2 P_{M1,2} = \psi_1^{MS(100)}(udu) \xi^{MA} \pi_{S1,S2}.$$  

(4.15)

Choosing $\pi^M$ yields a product of four $M$ irreps, which contains three copies of $S$; these can be labeled by the behavior of Dirac spin (i.e., the product of spin and quark parity) under permutation: $M \times M = S + A + M$,

$$2 P_{M3} = \psi_1^{MS(100)}(udu) \xi^{MA} \pi_{S1}$$

$$2 P_{M4} = \psi_1^{MS(100)}(udu) \xi^{MS} \pi_{MA}$$

$$2 P_{M5} = \psi_1^{MA(100)}(udu) \xi^{MA} \pi_{MA}.$$  

(4.16)

The first two yield, for Dirac spin, independent linear combinations of $A$ and $M$, and the third is a combination of $S$ and $M$. The corresponding Dirac structures are listed in Tab. 4.3; note that $2 P_{M1}$ and $2 P_{M3}$ have been mixed. To be explicit, the last operator is

$$N(2 P_{M5})_\alpha(x) = \epsilon^{abc} \frac{1}{\sqrt{2}} ( (D_i \tilde{u}^T_a(x) C \gamma_4 \tilde{d}_b(x) - \tilde{u}^T_a(x) C \gamma_4 (D_i \tilde{d})_b(x)) \gamma_i \gamma_5 \tilde{u}_c(x))_\alpha.$$  

(4.17)

For $S = \frac{3}{2}$, the $\xi$ part is symmetric, and we can use the pattern from $2 S_{S}$ to get three operators:

$$4 P_{M1,2,3} = \psi_1^{MA(100)}(udu) \xi^S \pi_{S1,S2,MS}.$$  

(4.18)

Combining spin 1 from the first two quarks with the third quark yields a vector index $j$ and a spinor index; contracting this with $\gamma_j$ gives $S = \frac{1}{2}$, which we don’t want, so we project onto $S = \frac{3}{2}$ using $\delta_{ij} - \frac{1}{3} \gamma_i \gamma_j$ (see Tab. 4.3).

Two derivatives can be applied to either the same quark or to different quarks. If
the derivatives are symmetrized yielding $L = 0$ and $L = 2$, then there are $S$ and $M$
combinations:

\[
\psi_{ij}^{S(200)} = \frac{1}{\sqrt{3}} \left( (D_iD_j)\phi^{(1)})\phi^{(2)}\phi^{(3)} + \phi^{(1)}(D_iD_j)\phi^{(2)}\phi^{(3)} + \phi^{(1)}\phi^{(2)}(D_iD_j)\phi^{(3)} \right)
\]

\[
\psi_{ij}^{S(110)} = \frac{1}{\sqrt{3}} \left( (D_i\phi^{(2)})(D_j)\phi^{(3)} + (D_i\phi^{(1)})\phi^{(2)}(D_j)\phi^{(3)} \right)
\]

\[
\psi_{ij}^{MS(200)} = \frac{1}{\sqrt{6}} \left( (D_iD_j)\phi^{(1)})\phi^{(2)}\phi^{(3)} + \phi^{(1)}(D_iD_j)\phi^{(2)}\phi^{(3)} - 2\phi^{(1)}\phi^{(2)}(D_iD_j)\phi^{(3)} \right)
\]

\[
\psi_{ij}^{MS(110)} = \frac{1}{\sqrt{6}} \left( (D_i\phi^{(2)})(D_j)\phi^{(3)} + (D_i\phi^{(1)})\phi^{(2)}(D_j)\phi^{(3)} - 2(D_i\phi^{(1)})(D_j)\phi^{(2)}\phi^{(3)} \right)
\]

\[
\psi_{ij}^{MA(200)} = \frac{1}{\sqrt{2}} \left( ((D_iD_j)\phi^{(1)})\phi^{(2)}\phi^{(3)} + \phi^{(1)}(D_iD_j)\phi^{(2)}\phi^{(3)} \right)
\]

\[
\psi_{ij}^{MA(110)} = \frac{1}{\sqrt{2}} \left( (D_i\phi^{(2)})(D_j)\phi^{(3)} - (D_i\phi^{(1)})\phi^{(2)}(D_j)\phi^{(3)} \right)
\]

Noting that $D_i\phi^{(j)}$ behaves like $(r_j)_i$, we find the combinations which don’t affect the center of mass ($R$):

\[
\psi_{ij}^{S(2)} = \frac{1}{\sqrt{2}} \left( \psi_{ij}^{S(200)} - \psi_{ij}^{S(110)} \right)
\]

\[
\psi_{ij}^{MS(2)} = \frac{1}{\sqrt{3}} \left( \psi_{ij}^{MS(200)} + 2\psi_{ij}^{MS(110)} \right)
\]

\[
\psi_{ij}^{MA(2)} = \frac{1}{\sqrt{3}} \left( \psi_{ij}^{MA(200)} + 2\psi_{ij}^{MA(110)} \right) \quad (4.19)
\]

which behave like $\rho_i\rho_j + \lambda_i\lambda_j$, $\rho_i\rho_j - \lambda_i\lambda_j$, and $\rho_i\lambda_j$, respectively. We get $L = 0$ by contracting $i$ with $j$; using $\psi_{ij}^{S(2)} \equiv \psi_{ii}^{S(2)}$, there are three operators as was the case for zero derivatives:

\[
2S'_{S1,2,3} = \psi_0^{S(2)}(udu)\xi_{\pi^+}^{MA,S1,S2,MS} \quad (4.20)
\]

With $\psi_{ij}^{MS(2),MA(2)} \equiv \psi_{ii}^{MS(2),MA(2)}$, there are five operators like with $2P_M$:

\[
2S_{M1,2,3} = \psi_0^{MS(2)}(udu)\xi_{\pi^+}^{MA,S1,S2,MS}
\]

\[
2S_M4 = \psi_0^{MS(2)}(udu)\xi_{\pi^+}^{MA}
\]

\[
2S_M5 = \psi_0^{MA(2)}(udu)\xi_{\pi^+}^{MA} \quad (4.22)
\]

For $L = 2$, we take the traceless part, e.g., $\psi_{ij}^{S(2)} \equiv \psi_{ij}^{S(2)} - \frac{1}{3}\delta_{ij}\psi_{kk}^{S(2)}$. We also need $S = \frac{3}{2}$, which means that the spin degrees of freedom are symmetric. If the spatial part
is also symmetric, then the quark parity part must have mixed symmetry, yielding
just one operator,

\[ 4D_S = \psi_2^{S(2)}(udu) \xi^S \pi_{+}^{MA}, \]  

with corresponding spinor structure \((u^T C \gamma_i \gamma_5 d) \gamma_j u\), where the indices \(ij\) are contracted with the corresponding derivatives. Taking the mixed-symmetry spatial part yields three operators,

\[ 4D_{M1,2,3} = \psi_2^{MA(2)}(udu) \xi^S \pi_{+}^{S1,S1,MS}, \]

where, again, the spinor structures listed in Tab. 4.3 have indices \(ij\) that are contracted with the derivatives.

If two derivatives are applied antisymmetrically to the same quark, this corresponds to including a gluon in the operator, which we leave out from this set. Applying them to different quarks yields \(A\) and \(M\) combinations with \(L = 1, 2\),

\[ \psi_1^{A(110)} = \frac{\epsilon^{ijk}}{\sqrt{3}} \left( \phi^{(1)}(D_j \phi^{(2)})(D_k \phi^{(3)}) + (D_k \phi^{(1)})(D_j \phi^{(2)})(D_i \phi^{(3)}) \right), \]

\[ \psi_1^{MA(110)} = \frac{\epsilon^{ijk}}{\sqrt{6}} \left( \phi^{(1)}(D_j \phi^{(2)})(D_k \phi^{(3)}) + (D_k \phi^{(1)})(D_j \phi^{(2)})(D_i \phi^{(3)}) \right) - 2(D_j \phi^{(1)})(D_k \phi^{(2)})(D_i \phi^{(3)}), \]

\[ \psi_1^{MS(110)} = \frac{\epsilon^{ijk}}{\sqrt{2}} \left( \phi^{(1)}(D_j \phi^{(2)})(D_k \phi^{(3)}) + (D_k \phi^{(1)})(D_j \phi^{(2)})(D_i \phi^{(3)}) \right), \]

which behave like \(\rho \times \lambda, \rho \times R,\) and \(\lambda \times R,\) respectively. Keeping just the first one, with \(S = \frac{1}{2}\) there are three operators,

\[ 2P_{A1,2,3} = \psi_1^{A(110)}(udu) \xi^S \pi_{+}^{S1,S1,MS}. \]

For \(S = \frac{3}{2}\), we need \(\pi^M\), so there is just one operator,

\[ 4P_A = \psi_1^{A(110)}(udu) \xi^S \pi_{+}^{MS}. \]

(again, see Tab. 4.3).

In lattice QCD, there is an additional complication: because there is only octahedral rotational symmetry rather than \(O(3)\), \(L = 2\) is a reducible representation. This means that the symmetric part of a two-component tensor \(T_{ii}\) can be decomposed into the usual singlet \(T_{ii}\) as well as the \(3'\) and 2 representations:

\[ T^{(3')} = \begin{pmatrix} \frac{1}{\sqrt{2}}(T_{23} + T_{32}) \\ \frac{1}{\sqrt{2}}(T_{13} + T_{31}) \\ \frac{1}{\sqrt{2}}(T_{12} + T_{21}) \end{pmatrix}, \quad T^{(2)} = \begin{pmatrix} \frac{1}{\sqrt{6}}(T_{11} - T_{22}) \\ \frac{1}{\sqrt{2}}(T_{11} + T_{22} - 2T_{33}) \end{pmatrix}. \]

For the \(4D_{\Pi}\) operators, each can be decomposed into two independent operators, \(4D_{\Pi}^{(3')}\) and \(4D_{\Pi}^{(2)}\), from the two parts of the contraction with the traceless symmetric \(T_{ij}\).

A similar set of interpolating operators was constructed in Refs. \[ \text{BEF}^{+05b}, \text{BEF}^{+05a}, \]

based on the octahedral group. The same set of operators presented
Table 4.3: Nucleon interpolating operators with up to two derivatives. The number of terms indicates how many terms are needed to express the operator in the generic form of Eq. 4.29; the $L = 2$ operators have two numbers for the two operators into which they are decomposed according to the lattice symmetry group.
here was also constructed independently in Ref. [EDRW11], although there the $^{2}S_{S}$ operators were omitted.

### 4.1.2 Two-point correlators

Generically, these interpolating operators can be written as

$$N_{\delta} = \sum_{n} \epsilon^{abc} \left( (u_{1}^{n})_{a}^{T} S_{n}^{n} (d^{n})_{b} \right) (R_{n}^{n} u_{2}^{n})_{c} \delta,$$

(4.29)

where $q^{n}$ is one of $\tilde{q}, D_{i} \tilde{q}, D_{i}^{2} \tilde{q}, D_{2,i}^{2} \tilde{q}, D_{3,i}^{2} \tilde{q},$ (4.30)

and $S_{n}$ and $R_{n}$ are matrices. Whereas the standard nucleon two-point correlator can be computed using a single smeared-to-all lattice quark propagator, two-point correlators using this larger set of operators require up to ten propagators, computed with the standard smeared source as well as covariant derivatives of it.

The number of terms for each operator is listed in Tab. [4.3] the computer time required for contractions scales with the product of the number of terms of the source operator with that of the sink operator. Because of this, in a small study it is impractical to compute the full matrix of zero-momentum two-point correlators between all pairs of operators,

$$C_{ij}(t) = \sum_{x} T_{\delta \delta}(\delta \delta(x,t) \tilde{N}_{\delta}^{(j)}(0,0)).$$

(4.31)

In Ref. [EDRW11], this was computed using the distillation method [PBF+09], for which there is a large initial cost but the cost of doing contractions is smaller. Although it is possible to use the distillation method to compute three-point correlators for operator matrix elements, this has yet to be done in practice, and it would be challenging to compute the large range of observables that are accessible with a small marginal cost when using the sequential sink method.

We study these operators using on an ensemble of gauge configurations with $m_{\pi} \approx 200$ MeV, $a = 0.116$ fm, and lattice volume $32^{3} \times 48$ (see Chapter [5]).

We begin with an initial study of the less-expensive operators by computing 201 measurements of the first row and column and the diagonal of $C_{ij}$, where the first operator is the standard one, $^{2}S_{S}$. It turns out that $C_{i0}$ is generally less noisy than $C_{0i}$, so we use only the former, and find the latter from Hermiticity of $C_{ij}$.

Each operator is evaluated by solving the generalized eigenvalue problem, Eq. [4.5] for the two-operator system consisting of that operator and the standard one. We compare the resulting effective mass, $m_{\text{eff}}(t, t_{0})$, with $m_{0}^{0}(t)$ from the standard operator:

$$am_{\text{eff}}(t, t_{0}) = \frac{\lambda(t, t_{0})}{\lambda(t + a, t_{0})} \quad am_{\text{eff}}^{0}(t) = \frac{C_{00}(t)}{C_{00}(t + a)}.$$

(4.32)

If the additional operator is effective at helping to isolate the ground-state, then the two-operator effective mass should reach a plateau more rapidly, and therefore we plot
the ratio
\[ R(t) = \frac{m_{\text{eff}}(t, t)}{m_{\text{eff}}(t)}, \]
which should be less than 1 at small \( t \). This is shown in Fig. 4-1; adding a second operator yields at most a very slight improvement over the standard tuned operator.

A subset of seven operators was selected for further study, based on a combination of cost and hints of usefulness from \( R(t) \). For these, we compute 411 measurements of the full two-point correlator matrix. The resulting effective mass is plotted in Fig. 4-2 along with \( m_{\text{eff}}^0 \). It is clear that \( m_{\text{eff}} \) from this 7-operator system approaches a plateau faster than the standard operator, but the difference is small. Because of the high cost and unclear benefits, we decided to not use these operators for computing three-point correlators and matrix elements, and instead pursue more-economical methods of studying systematic errors from excited states.

### 4.2 Ground-state matrix elements from multiple source-sink separations

The simplest way of improving on the standard calculation described at the beginning of this chapter is to compute three-point correlators using multiple source-sink separations. At the very least, this should provide a clear signal indicating which observables are affected by significant excited-state contaminations. Furthermore, it may be possible to
make use of multiple time-separations to remove much of the contribution from excited states. In this section, we describe different methods of computing matrix elements and then apply them to a high-precision test case where we computed three-point correlators using five source-sink separations.

### 4.2.1 Ratio method

We label proton states as $|\vec{p}, \lambda\rangle$ and use the normalization $\langle \vec{p}', \lambda'|\vec{p}, \lambda\rangle = 2EL_z\delta_{\vec{p}, \vec{p}'}\delta_{\lambda, \lambda'}$. Parameterizing the overlap of our interpolating operator with the ground-state proton as $\langle \Omega|N_\alpha(\vec{x})|\vec{p}, \lambda\rangle = \sqrt{Z(\vec{p})}u_\alpha(\vec{p}, \lambda)e^{i\vec{p} \cdot \vec{x}}$, from Eqs. 3.28 and 3.29 at zero temperature we obtain

$$C_{2pt}(\vec{p}, t) = \frac{Z(\vec{p})e^{-E(\vec{p})t}}{2E(\vec{p})}\text{Tr}[\Gamma_{\text{pol}}(i\gamma + m_N)] + O(e^{-\Delta E_{10}(\vec{p})t}) \quad (4.34)$$

$$C_{3pt}^{\Omega}(\vec{p}, \vec{p}', \tau, T) = \frac{Z(\vec{p})Z(\vec{p}')e^{-E(\vec{p})\tau - E(\vec{p}')(T-\tau)}}{4E(\vec{p})E(\vec{p}')}\sum_{\lambda, \lambda'} \bar{u}(\vec{p}, \lambda)\Gamma_{\text{pol}}u(\vec{p}', \lambda')\langle \vec{p}', \lambda'|\Omega|\vec{p}, \lambda\rangle + O(e^{-\Delta E_{10}(\vec{p})\tau}) + O(e^{-\Delta E_{10}(\vec{p}')(T-\tau)}), \quad (4.35)$$

where $\Delta E_{10}(\vec{p})$ is the energy gap between the ground and lowest excited state with momentum $\vec{p}$. To cancel the overlap factors and the dependence on Euclidean time, we
compute the ratios,
\[
R^{\text{C}^0}(\tau, T) \equiv \frac{C_{3\text{pt}}^{\text{C}^0}(\vec{p}, \vec{p}', \tau, T)}{\sqrt{C_{2\text{pt}}(\vec{p}, T) C_{2\text{pt}}(\vec{p}', T)}} \frac{\sqrt{C_{2\text{pt}}(\vec{p}, T - \tau) C_{2\text{pt}}(\vec{p}', \tau)}}{C_{2\text{pt}}(\vec{p}, T - \tau) C_{2\text{pt}}(\vec{p}', \tau)} = \sum_{\lambda, \lambda'} \bar{u}(\vec{p}, \lambda) \Gamma_{\text{pol}} u(\vec{p}', \lambda') \langle p', \lambda' | O^q | p, \lambda \rangle \sqrt{2E(\vec{p}) (2E(\vec{p}) + m_N) \cdot 2E(\vec{p}') (2E(\vec{p}') + m_N) + O(e^{-\Delta E_{10}(\vec{p}) \tau}) + O(e^{-\Delta E_{10}(\vec{p}') (T-\tau})}. \tag{4.36}
\]

As a function of \(\tau \in [0, T]\) with fixed \(T\), the ratios produce a plateau with "tails" at both ends caused by excited states. In practice, for each fixed \(T\), we average over the central two or three points near \(\tau = T/2\), which allows for matrix elements to be computed with errors that decay asymptotically as \(e^{-\Delta E_{\text{min}} T/2}\), where \(\Delta E_{\text{min}} = \min\{\Delta E_{10}(\vec{p}), \Delta E_{10}(\vec{p}')\}\).

### 4.2.2 Summation method

Improved asymptotic behavior of excited-state contributions can be achieved by using the summation method [CKDMW10, BDS10]. Taking the sums of ratios yields
\[
S(T) \equiv \sum_{\tau = \tau_0}^{T - \tau_0} R(\tau, T) = c + TM + O(e^{-\Delta E_{\text{min}} T}), \tag{4.37}
\]
where \(c\) is independent of \(T\), and \(M\) contains the desired ground-state matrix element (we omit the first and last \(\tau_0 = 1\) points of each plateau). Thus finite differences, \((\delta T)^{-1}(S(T + \delta T) - S(T))\), yield the ground-state matrix element with excited-state contamination that asymptotically decays\(^1\) as \(e^{-\Delta E_{\text{min}} T}\).

### 4.2.3 Generalized pencil-of-function method

With three-point correlators computed using a single interpolating operator and at least three source-sink separations, we are able to make use of the variational method via the generalized pencil-of-function (GPoF) method [AO11]. This is based on the recognition that if \(N(t)\) is our interpolating operator for the nucleon, then the time-displaced operator
\[
N^\delta(t) \equiv e^{H\delta} N(t) e^{-H\delta} = N(t + \delta) \tag{4.38}
\]
When there is degeneracy between initial and final states, such as for forward matrix elements or in the Breit frame, the leading error here and in Eq. 4.37 is \(O(T e^{-\Delta E_{10} T})\), which comes from the subleading \(O(e^{-\Delta E_{10} T})\) error in Eq. 4.36 for the ratio method.

\[^1\text{When there is degeneracy between initial and final states, such as for forward matrix elements or in the Breit frame, the leading error here and in Eq. 4.37 is } O(T e^{-\Delta E_{10} T}), \text{ which comes from the subleading } O(e^{-\Delta E_{10} T}) \text{ error in Eq. 4.36 for the ratio method.}\]
is a linearly independent interpolating operator for the nucleon. This enables us to construct a matrix of two-point functions,

\[
C_{2pt}(t) = \begin{pmatrix}
\langle N(t)\bar{N}(0) \rangle & \langle N^\delta(t)\bar{N}(0) \rangle \\
\langle N(t)\bar{N}^\delta(0) \rangle & \langle N^\delta(t)\bar{N}^\delta(0) \rangle
\end{pmatrix} = \begin{pmatrix}
C_{2pt}(t) & C_{2pt}(t + \delta) \\
C_{2pt}(t + \delta) & C_{2pt}(t + 2\delta)
\end{pmatrix},
\]

(4.39)

using our ordinary two-point function \(C_{2pt}(t)\). By solving the generalized eigenvalue problem, Eq. [4.5] we can find eigenvectors \(v(t_0, t)\) that asymptotically give linear combinations of \(N\) and \(N^\delta\) which have zero overlap with the first excited state. Then using also the matrix of three-point functions,

\[
C_{3pt}(\tau, T) = \begin{pmatrix}
\langle N(T)\mathcal{O}(\tau)\bar{N}(0) \rangle & \langle N^\delta(T)\mathcal{O}(\tau)\bar{N}(0) \rangle \\
\langle N(T)\mathcal{O}(\tau)\bar{N}^\delta(0) \rangle & \langle N^\delta(T)\mathcal{O}(\tau)\bar{N}^\delta(0) \rangle
\end{pmatrix} = \begin{pmatrix}
C_{3pt}(\tau, T) & C_{3pt}(\tau, T + \delta) \\
C_{3pt}(\tau + \delta, T + \delta) & C_{3pt}(\tau + \delta, T + 2\delta)
\end{pmatrix},
\]

(4.40)

we compute two-point and three-point functions using a particular linear combination:

\[
C_{2pt}^{\text{GPoF}}(t) = v^\dagger C_{2pt}(t)v \quad C_{3pt}^{\text{GPoF}}(\tau, T) = v^\dagger C_{3pt}(\tau, T)v,
\]

(4.41)

and then proceed with the usual ratio-plateau analysis. This requires computing three-point functions at three equally spaced source-sink separations.

In practice, for each class of lattice momenta \(\vec{p}\) equivalent under the group of lattice rotations and reflections, we average the two-point correlators \(C_{2pt}(t, \vec{p})\) and then use the GPoF method and solve the generalized eigenvalue problem. This produces a different linear combination of the original and the time-displaced nucleon operator for each class of equivalent lattice momenta. Although the lowest-lying excited state can be asymptotically removed by appropriately increasing \(t_0\) and \(t\) as \(\tau\) and \(T - \tau\) are increased [BDMvH+09], we instead find the eigenvector using fixed values of \(t_0\) and \(t\), which only reduces the contribution from the leading excited state in \(C_{2pt}(t)\).

### 4.2.4 High-precision test calculations

To study excited-state contaminations and ways of removing them, we perform calculations on a lattice QCD gauge field ensemble generated by USQCD, with 2+1 flavors of Wilson-clover fermions coupled to gauge fields that have been smeared using one level of stout smearing. This ensemble has lattice volume \(32^3 \times 96\), lattice spacing \(a \approx 0.114\) fm, and pion mass \(m_\pi \approx 317\) MeV. We compute 24672 measurements on 1028 gauge configurations to achieve high precision, using source-sink separations \(T/a \in \{6, 8, 10, 12, 14\}\), and two sink momenta: \(\vec{p} = \vec{0}\) and \(\vec{p} = \frac{2\pi}{L_s}(-1, 0, 0)\). We also restrict the source momentum to be no larger than \(\frac{2\pi}{L_s}(1, 1, 1)\); this yields eleven different momentum transfers, which are listed in Tab. [4.4].

We compute matrix elements in the following ways:

1. Using the ratio method, averaging over the three central points of each plateau. This yields one result for each of the five source-sink separations.
Table 4.4: Representative source and sink momenta $\vec{p} = \frac{2\pi}{L_s} \vec{n}$ for each of the eleven different momentum transfers at which we compute matrix elements.

2. With the summation method, using finite differences from sums at adjacent source-sink separations; i.e., with $\delta T = 2a$. This yields one result for each of the four pairs of adjacent source-sink separations.

3. Using the GPoF method, using a shift of the interpolating operator by $\delta = 2a$ to combine three adjacent source-sink separations. We use fixed eigenvectors from solving the generalized eigenvalue problem with $(t_0, t) = (a, 2a)$; the resulting two-point correlators are compared in Fig. 4-3. By $t = 2a$, $C_{2pt}^{\text{GPoF}}(t, \vec{p})$ is already consistent with a single exponential, so with the current level of statistics there is no benefit to finding the eigenvector at larger time-separations. Applying the ratio-plateau method to $C_{2pt}^{\text{GPoF}}$ and $C_{3pt}^{\text{GPoF}}$ yields one result for each of the three effective source-sink separations.

We have not yet performed a calculation for the renormalization of operators on this ensemble; therefore, the results presented in this section are unrenormalized, “bare” quantities. This does not affect the study of excited-state contributions.

The isovector Dirac and Pauli form factors are shown for the set of eleven momentum transfers in Fig. 4-4. At $Q^2 = 0$, $F_1^v$ shows statistically significant excited-state effects at the sub-percent level, which we interpret as a discretization effect since, in the continuum limit, this corresponds to a conserved charge: the third component of isospin $I_3$. As $Q^2$ increases, the effect of removing excited states is to decrease the value of $F_1$; this effect grows with $Q^2$ and thus removing excited states increases the computed value of the isovector Dirac radius $(r_2^v)$. The GPoF method produces a generally stable result that is consistent with results from the ratio method when using the largest two or three source-sink separations. The benefit of the summation method can be seen clearly: calculations performed using $T/a \in \{6, 8\}$ can produce either the first two ratio points, which suffer from significant excited-state contamination, or they can be combined to produce the first summation point, which is consistent with the GPoF results.
Figure 4-3: Two-point correlators $C_{2pt}(t, \vec{p})$ and $C^{GPoF}_{2pt}(t, \vec{p})$, divided by their ground-state contributions, as determined from a one-state fit. Correlators are averaged over equivalent momenta. The GPoF correlators are shifted to compare the chosen linear combination of $N$ and $N^{\delta}$ against $N^{\delta}$ alone.
The isovector Pauli form factor $F_2^v$ shows large excited-state effects at the smallest values of $Q^2$. These become much smaller at larger values of $Q^2$, with the result that removing excited states increases the computed values of both the isovector anomalous magnetic moment $\kappa^v$ and the isovector Pauli radius $(r_2^v)^v$. On first impression, it appears that excited-state effects are not at all under control for $F_2^v$ at the smallest $Q^2$, since the three methods of computing matrix elements all produce results that increase monotonically with source-sink separation without any sign of reaching a plateau. A more charitable interpretation of the figure is that, since the data are highly correlated, the increase at the largest source-sink separations may simply be a fluctuation. The two first summation points are consistent with one another, suggesting that this may be a plateau.

We show the isovector axial and induced pseudoscalar form factors in Fig. 4-5. At $Q^2 = 0$ (i.e., for $g_A$) and at small $Q^2$, $G_A^v$ increases with source-sink separation, and as $Q^2$ is increased, the effect changes direction and $G_A^v$ starts to decrease with source-sink separation. The result is that removing excited states tends to increase the computed values of both $g_A$ and the isovector axial radius $(r_A^v)^v$. These excited-state effects are relatively mild when compared with isovector induced pseudoscalar form factor $G_P^v$, which shows very large effects at small $Q^2$. Neither the ratio method nor the GPoF method indicate that a plateau has been reached. The summation method may have a plateau starting with the second point, which is also consistent with the other two methods, when using the largest source-sink separation.

Figure 4-6 shows form factors of the isovector quark energy-momentum operator, $A_{20}^v$ and $B_{20}^v$ (the third form factor, $C_{2}^v$, is generally consistent with zero and has less clear excited-state effects). Both of these show excited-state effects that are roughly independent of $Q^2$, with $A_{20}^v$ suffering from larger effects than $B_{20}^v$. As a result, calculated values of both the isovector average momentum fraction $\langle x \rangle_{u-d}$ and total quark angular momentum $J^{u-d}$ will tend to decrease as excited states are removed. For the first eight momentum transfers, the ratio and GPoF calculations of $A_{20}^v$ both decrease monotonically with source-sink separation, suggesting that a plateau has not yet been reached.

The data in this section show the effectiveness of the summation method, particularly at source-sink separations where the ratio method does not produce stable results. This helps to motivate the use of the summation method for many of the primary results in the next chapter. Results from calculations done using this ensemble will continue to be shown, including some observables not shown in this section, in order to assist the interpretation of the less-precise calculations in the next chapter.
Figure 4-4: Isovector Dirac and Pauli form factors $F_1^v(Q^2)$ and $F_2^v(Q^2)$ on the USQCD ensemble, computed using the ratio, GPoF, and summation methods. Each method is shown with multiple points at each $Q^2$, corresponding to different source-sink separations increasing from left to right.
Figure 4-5: Isovector axial and induced pseudoscalar form factors $G_A^v(Q^2)$ and $G_P^v(Q^2)$ on the USQCD ensemble; see the caption of Fig. 4-4.
Figure 4-6: Isovector generalized form factors $A_{20}^v(Q^2)$ and $B_{20}^v(Q^2)$ on the USQCD ensemble; see the caption of Fig. 4-4.
Chapter 5

Nucleon structure near the physical pion mass

In this chapter, we present results from nucleon structure calculations using the Budapest-Marseille-Wuppertal (BMW) action with 2+1 flavors of tree-level clover-improved Wilson fermions that couple to double-HEX-smeared gauge fields (see Ref. [DFH+11]). The ensembles used have pion masses that reach as low as 149 MeV, which is just 10% above the physical value of 134.8 MeV in the isospin limit [CDJ+11].

On each ensemble, we compute the three-point correlators using three source-sink separations: \( T/a \in \{8, 10, 12\} \) for the coarse \((a = 0.116 \text{ fm})\) ensembles and \( T/a \in \{10, 13, 16\} \) for the one fine \((a = 0.09 \text{ fm})\) ensemble. The ten ensembles are listed in Tab. 5.1 and summarized in Fig. 5-1.

We renormalize the vector current using the fact that \( F_v(0) = 1 \). Other operators are renormalized using the Rome-Southampton method [MPS+95], to renormalize in the \( \overline{\text{MS}} \) scheme at \( \mu = 2 \text{ GeV} \) via perturbative matching to the \( RI'/MOM \) scheme in which we renormalize using a nonperturbative calculation on the lattice. Details of this are given in Ref. [GNP+12]; for the scalar quark bilinear, we use the renormalization factors computed in Ref. [DFH+11].

With three source-sink separations and noisier calculations than in Section 4.2.4,

<table>
<thead>
<tr>
<th>( m_\pi ) (MeV)</th>
<th>( a ) (fm)</th>
<th>( L_s^3 \times L_t )</th>
<th>( m_\pi L_s )</th>
<th>( m_\pi L_t )</th>
<th>( N_{\text{conf}} )</th>
<th>( N_{\text{meas}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>149(1)</td>
<td>0.116</td>
<td>( 48^3 \times 48 )</td>
<td>4.2</td>
<td>4.2</td>
<td>646</td>
<td>7752</td>
</tr>
<tr>
<td>202(1)</td>
<td>0.116</td>
<td>( 32^3 \times 48 )</td>
<td>3.8</td>
<td>5.7</td>
<td>457</td>
<td>5484</td>
</tr>
<tr>
<td>253(1)</td>
<td>0.116</td>
<td>( 32^3 \times 96 )</td>
<td>4.8</td>
<td>14.3</td>
<td>202</td>
<td>2424</td>
</tr>
<tr>
<td>254(1)</td>
<td>0.116</td>
<td>( 32^3 \times 48 )</td>
<td>4.8</td>
<td>7.2</td>
<td>420</td>
<td>5040</td>
</tr>
<tr>
<td>254(1)</td>
<td>0.116</td>
<td>( 24^3 \times 48 )</td>
<td>3.6</td>
<td>7.2</td>
<td>419</td>
<td>10056</td>
</tr>
<tr>
<td>252(2)</td>
<td>0.116</td>
<td>( 24^3 \times 24 )</td>
<td>3.6</td>
<td>3.6</td>
<td>1125</td>
<td>6750</td>
</tr>
<tr>
<td>303(2)</td>
<td>0.116</td>
<td>( 24^3 \times 48 )</td>
<td>4.3</td>
<td>8.6</td>
<td>128</td>
<td>768</td>
</tr>
<tr>
<td>317(2)</td>
<td>0.093</td>
<td>( 32^3 \times 64 )</td>
<td>4.6</td>
<td>9.3</td>
<td>103</td>
<td>824</td>
</tr>
<tr>
<td>356(2)</td>
<td>0.116</td>
<td>( 24^3 \times 48 )</td>
<td>5.0</td>
<td>5.0</td>
<td>127</td>
<td>762</td>
</tr>
<tr>
<td>351(2)</td>
<td>0.116</td>
<td>( 24^3 \times 24 )</td>
<td>5.0</td>
<td>10.1</td>
<td>420</td>
<td>2520</td>
</tr>
</tbody>
</table>

Table 5.1: Lattice ensembles using the BMW action.
we compute matrix elements in the following ways:

1. Using the ratio method, averaging over the three central points of each plateau. This yields one result for each of the three source-sink separations.

2. With the summation method, the finite difference between the two larger source-sink separations is too noisy to be useful. Therefore, we fit a line to the sums at the three source-sink separations to yield one result.

3. Using the GPoF method as in Section 4.2.4, yielding one result because there is now just one effective source-sink separation.

Except for the largest volume, we use source momenta up to \( \frac{2\pi}{L_s}(1,1,1) \). On the largest volume, we include source momenta as large as \( \frac{2\pi}{L_s}(2,1,1) \).

This set of ensembles allows for control over, or study of, various sources of systematic error. In roughly decreasing order of the level of control that we can achieve:

**Quark masses** For all ensembles, the strange quark mass is near the physical value. The smallest light quark mass corresponds to a pion mass that is just 10\% above the physical pion mass. This allows for either a direct comparison of the \( m_\pi = 149 \text{ MeV} \) ensemble with experiment, or a comparison after a mild extrapolation to the physical point.
Excited states Using the ratio method with three different source-sink separations allows for clear identification of observables where excited-state contamination is a problem. In addition, as studied in Section 4.2.4, the summation method is reasonably effective at removing the contributions from excited states, and the GPoF method is also an improvement over the standard ratio method.

Finite volume In general, finite-volume effects are expected to be small with $m_\pi L_s \gtrsim 4$, which is satisfied by most of the ensembles. Furthermore, the $24^3 \times 48$ and $32^3 \times 48$ ensembles near $m_\pi = 250$ MeV differ only in their spatial volume, which allows for a controlled check for finite-volume effects.

Finite temperature Most of these ensembles have the same time extent, which corresponds to a temperature of 35 MeV. It is more common to vary the time extent with the spatial extent such that $L_t = 2L_s$, so that both are larger at smaller $m_\pi$. At lower pion masses, the fixed temperature means that it becomes easier to thermally excite a pion, which could have unwanted influence on the results. On the other hand, the three different time extents $L_t/a \in \{24, 48, 96\}$ used for the ensembles near $m_\pi = 250$ MeV are useful for identifying possible thermal effects.

Discretization The one ensemble with a finer lattice spacing allows for a consistency check, but this set of ensembles is insufficient for taking a continuum limit or having some careful control over discretization effects.

Comparing with the recent lattice QCD calculations listed in Tab. 3.1, we see that this is the only calculation done with such a near-physical pion mass in a large volume. Furthermore, most calculations do not devote such resources to studying excited-state effects, and never at a near-physical pion mass.

Two ensembles will be the main ones studied: the $48^3 \times 48, m_\pi = 149$ MeV ensemble because it is close to the physical pion mass, and the $32^3 \times 48, m_\pi = 254$ MeV ensemble because it has the smallest statistical errors.

We will also perform extrapolations to the physical pion mass using chiral perturbation theory (ChPT), generally by fitting to calculations done on the ensembles with the smallest pion masses and largest volumes (the first four listed in Tab. 5.1). These are not the main focus of this thesis, so the relevant expressions are included in Appendix A. We will use results from phenomenology to constrain many of the parameters; therefore, the extrapolated observables are not fully ab initio results. The extrapolations will serve both to test the compatibility of the lattice data with ChPT and measurements from experiment, and to indicate the dependence on pion mass in the chiral regime more clearly than shown by the noisy lattice calculations.

5.1 Isovector vector form factors

The isovector Dirac and Pauli form factors are shown in Figs. 5-2 and 5-3 for the two main ensembles, computed using the different methods discussed above. On the
near-physical ensemble, there is a trend for \( F_v^1 \) to decrease and \( F_v^2 \) to increase when going from the shortest to the middle source-sink separation. This is consistent with what was seen more clearly on the \( m_\pi \approx 317 \text{ MeV} \) ensemble in Section 4.2.4. The summation and GPoF methods produce results with similar errors, but (except for the first two points) the summation values for \( F_v^v \) lie consistently lower, which suggests that excited-state effects are not fully controlled on this ensemble. The dependence on source-sink separation for the \( m_\pi = 254 \text{ MeV} \) ensemble is qualitatively similar, but the effect is weaker.

Determining the Dirac and Pauli radii and the anomalous magnetic moment from these \( F_{1,2}(Q^2) \) data requires fitting and interpolating the slope at \( Q^2 = 0 \) (for \( F_1 \)), or extrapolating the slope and value at \( Q^2 = 0 \) (for \( F_2 \)). We fit a two-parameter dipole function,

\[
F(Q^2) = \frac{F(0)}{\left(1 + \frac{Q^2}{m_D^2}\right)^2},
\]

(5.1)
to the range \( 0 \leq Q^2 \leq 0.5 \text{ GeV}^2 \), for each ensemble. Because the data have large errors, the fits work well and there is no sign of deviation from dipole behavior except when using the shortest source-sink separation.

The resulting Dirac radius is shown in Fig. 5-4. The lattice calculations lie systematically below the experimental points, but it is clear that much of this discrepancy is due to excited-state effects. These are particularly large on the \( m_\pi = 149 \text{ MeV} \) ensemble, which shows the same pattern as the high-precision calculations done on the USQCD ensemble: the GPoF result is nearly the same as the \( T = 1.4 \text{ fm} \) ratio result, and the summation method yields a larger Dirac radius. Comparing the \( 32^3 \times 48 \) and \( 24^3 \times 48 \) ensembles with \( m_\pi \approx 250 \text{ MeV} \), we do not find any significant finite-volume effects.

A fit and extrapolation using Eq. A.4 with one free parameter is shown in Fig. 5-5. Fitting to the summation data works well, with \( \chi^2/\text{dof} = 1.7/3 \), and the extrapolated value is consistent with experiment. Using the GPoF data (\( \chi^2 = 7.5 \)) or the ratio data (\( \chi^2 > 14 \)) yields much worse fits.

In Fig. 5-6, we show the isovector anomalous magnetic moment, normalized relative to the physical magneton, rather than using the ensemble-dependent nucleon mass as in Eq. 3.9

\[
\kappa_{\text{norm}}^v = \frac{\kappa_{N}^\text{phys}}{m_N^\text{lat}} F_{2}^{v,\text{lat}}(0).
\]

(5.2)

We again see that the influence of excited states is qualitatively the same on the \( m_\pi = 149 \text{ MeV} \) ensemble as on the high-precision USQCD ensemble; however, unlike for the Dirac radius, the rest of the BMW-action ensembles don’t show a clear trend of excited-state effects. The ensembles with smaller volumes also suffer from much larger statistical errors. This is because the Pauli form factor must be extrapolated to zero momentum transfer, and the smallest available \( Q^2 \) in a periodic box is \( Q_{\text{min}}^2 \approx \left(\frac{2\pi}{L}\right)^2 \), so a longer extrapolation is required when using a smaller volume. Therefore, to check for finite-volume effects, we compare the form factor \( F_{2}^{v}(Q^2) \) on the \( 24^3 \times 48 \) and \( 32^3 \times 48 \) ensembles at \( m_\pi \approx 250 \text{ MeV} \) in Fig. 5-7. There does not appear to be a
Figure 5-2: Comparison of the isovector Dirac and Pauli form factors, computed using different methods, on the $m_\pi = 149$ MeV ensemble.
Figure 5-3: Comparison of the isovector Dirac and Pauli form factors, computed using different methods, on the $32^3 \times 48$, $m_\pi = 254$ MeV ensemble.
Figure 5-4: Isovector Dirac radius from dipole fits. The BMW ensembles are ordered by increasing pion mass. Ensembles with the same pion mass are ordered by decreasing four-dimensional lattice volume. The equivalent calculations done using the USQCD clover ensemble from Sec. 4.2.4 are shown on the far right. We also show two experimental points, where $(r_E^2)^p$ is taken from either the CODATA 2010 result [MTN12] used by the PDG [B+12] or the measurement from spectroscopy of muonic hydrogen [ANS+13]. Both points use the PDG value for $(r_E^2)^n$. 
Figure 5-5: Isovector Dirac radius from fits to $F_1^v(Q^2)$ computed using the summation method and chiral extrapolation to the physical pion mass. Points in red are included in the fit. On the left, the extrapolated values computed using other methods are also shown; see the legend of Fig. 5-4.
Figure 5-6: Isovector anomalous magnetic moment from dipole fits on the BMW and USQCD ensembles; see the caption of Fig. 5-4. The experimental value is taken from the 2012 PDG $^{12}$. The significant finite-volume effect, compared with the statistical errors.

Extrapolation of $\kappa_v^{\text{norm}}$ to the physical pion mass with two-parameter fits using Eq. A.5 is shown in Fig. 5-8. The fits to the points computed using summation, GPoF, and ratio with the larger two source-sink separations are all good, with $\chi^2/\text{dof} < 1$. The summation, GPoF, and $T = 1.4 \text{ fm}$ ratio-method extrapolated values are consistent with one another and with experiment, suggesting that excited states are reasonably under control. The extrapolated points using the ratio method with the lower two source-sink separations lie below the experimental value and approach it as the source-sink separation is increased and excited-state contaminations are removed.

We see behavior in the isovector Pauli radius similar to that in the isovector anomalous magnetic moment; the former is shown in Fig. 5-9. In particular, the calculations done using the $m_\pi = 149 \text{ MeV}$ ensemble behave similarly to the high-precision calculations using the USQCD ensemble: $(r_2^2)^v$ increases with source-sink separation, the GPoF result is similar to the largest source-sink separation, and the summation result is still higher. The three $L_s = 32$ coarse BMW ensembles, however, do not follow this trend. Because of the previously-discussed difficulty of extrapolating to $Q^2 = 0$ when using smaller volumes, we refer the reader to the earlier discussion and Fig. 5-7 for evidence that finite-volume effects are not large.

In chiral perturbation theory, it is more natural to use the combination $\kappa_v^{\text{norm}} (r_2^2)^v$. Fitting and extrapolation of this quantity using Eq. A.6 with one free parameter is shown in Fig. 5-10. The fits are of good quality, with $\chi^2/\text{dof} < 1$, when using the
Figure 5-7: Isovector Pauli form factor, computed using the summation method, for the two volumes at $m_\pi = 254$ MeV. Data with nearby $Q^2$ are binned for clarity. The dipole fit to the larger-volume ensemble is also shown.

Figure 5-8: Isovector anomalous magnetic moment from fits to $F_2^v(Q^2)$ computed using the summation method and chiral extrapolation to the physical pion mass. Points in red are included in the fit. On the left, the extrapolated values computed using other methods are also shown; see the legend of Fig. 5-6.
Figure 5-9: Isovector Pauli radius from dipole fits on the BMW and USQCD ensembles; see the caption of Fig. 5-4. We show two experimental values, where the radii are taken either from the 2012 PDG $[^{12}B + 12]$ or from the dispersion analysis in Ref. $[^{12}LHMT2]$ (the difference mostly comes from different values of the proton magnetic radius).
Figure 5-10: Isovector Pauli radius multiplied by the anomalous magnetic moment, $\kappa_{\text{norm}}(r_2^2)$, from fits to $F_2^v(Q^2)$ computed using the summation method and chiral extrapolation to the physical pion mass. Points in red are included in the fit. On the left, the extrapolated values computed using other methods are also shown; see the legend of Fig. 5-9.
summation or GPoF data, or when using the largest source-sink separation. Except when using the summation method, the extrapolated values all agree with one another and lie below the experimental points. The extrapolated summation value is consistent with both of the experimental values. Unlike for \((r^2)^v\) and \(\kappa^v\), the extrapolated ratio points do not move toward experiment as the source-sink separation is increased; with the present statistics, it is possible that this is merely a fluctuation, but this may also hint at challenges in controlling excited-state errors in the isovector Pauli radius.

Noting that, when using the summation method, the anomalous magnetic moment and Pauli radius on the \(m_\pi = 149\) MeV ensemble are consistent with experiment, and the Dirac radius is close to the experimental points, we find that it is worth comparing the form factors themselves with experiment. In Fig. [5-11] we compare the experimentally-preferred isovector Sachs form factors,

\[
G_E^v(Q^2) = F_1^v(Q^2) - \frac{Q^2}{2m_N}F_2^v(Q^2) \tag{5.3}
\]

\[
G_M^v(Q^2) = F_1^v(Q^2) + F_2^v(Q^2), \tag{5.4}
\]

between this lattice ensemble and the phenomenological parameterization of experimental data in Ref. [ABGG09]. The lattice data agree rather well with experiment, which is not the case if one of the other methods for computing form factors is used, or when comparing data from ensembles with heavier pion masses; this strongly supports the argument that both near-physical pion masses and good control over excited states are essential for a realistic calculation.

### 5.2 Isovector axial form factors

The best-measured aspect of the nucleon axial form factors is the axial charge \(g_A \equiv G_A^v(0) = 1.2701(25)\), from beta decay experiments [B+12]; we show our calculations of it in Fig. [5-12]. Unlike the vector form factors, this shows very different behavior in the \(m_\pi = 149\) MeV ensemble, compared with the high-precision test case. On the latter ensemble, and on three of the four ensembles with \(m_\pi \approx 250\) MeV, the value of \(g_A\) increases with the source-sink separation, and the summation method yields the largest value. On a second group of ensembles—those with \(m_\pi = 149\) and 202 MeV, and the \(m_\pi \approx 250\) MeV ensemble with short time-extent—the value of \(g_A\) decreases with the source-sink separation. The relevance of the time extent of the ensembles at \(m_\pi \approx 250\) MeV suggests that this effect is caused by thermal states. The dominant thermal contribution comes from pions at zero momentum, with a weight that scales as \(e^{-m_\pi L_t}\) (see Eq. 3.29), and in fact the value of \(m_\pi L_t\) is smaller on the second group of ensembles, where \(g_A\) decreases with source-sink separation, than it is on the ensembles where \(g_A\) increases with source-sink separation. Although larger statistics are required on the ensemble with \(L_t/a = 24\) to confirm the effect, this strongly suggests that the axial charge is particularly affected by thermal contamination, and this also casts suspicion on the axial form factors in general, when computed on the ensembles with

\[1\] Such a calculation is currently in progress.
Figure 5-11: Isovector electric and magnetic form factors: points from using the summation method on the $m_\pi = 149$ MeV ensemble (data at nearby $Q^2$ are binned for clarity) and curves from the fit to experiment in Ref. [ABGG09].
Figure 5-12: Axial charge on the BMW and USQCD ensembles; see the caption of Fig. 5-4. The normalization used on the USQCD ensemble is arbitrary, as we have not computed a renormalization factor. The experimental value is taken from the 2012 PDG [B12].
Given that there appears to be a problem with $g_A$ due to thermal states on the ensembles with the two smallest pion masses, and the calculated values of $g_A$ on those ensembles lie well below the value from experiment, it is clear that a chiral extrapolation using those ensembles will not agree with experiment. Instead, we make use of the ensembles with larger pion masses and select those with $m_\pi L_t > 7$. Using a two-parameter fit with Eq. A.7, the extrapolation to the physical pion mass is shown in Fig. 5-13. The fits are all of reasonably good quality: with 4 degrees of freedom they have $\chi^2 = 7.7$ when using the shortest source-sink separation and $\chi^2 < 3$ for the other cases. The extrapolated value of $g_A$ increases toward the experimental point when going from the shortest to the middle source-sink separation, and the summation and GPoF results are consistent with experiment. In Ref. [CDMvH+12], the summation method was also used, and an extrapolation with pion masses between 277 and 540 MeV also achieved agreement with experiment for $g_A$. There, the lattice temporal extents all satisfied $m_\pi L_t \geq 8$, and the ratio-plateau method produced results lower than the summation method, which is the same behavior that we see in our data. Therefore, our conclusion regarding $g_A$ is that thermal effects are particularly important, but excited states must also be under control in order to agree with experiment. Because we have excluded the two ensembles with the smallest pion masses, this result depends much more strongly on chiral perturbation theory than
the results in the previous section; a calculation near the physical pion mass with a large time extent and reasonable control over excited states is necessary to remove the dependence on chiral perturbation theory and phenomenological input.

The isovector axial form factor $G_A^v(Q^2)$ is shown for the two main ensembles in Fig. 5-14. The $m_\pi = 254$ MeV ensemble shows behavior roughly similar to what we saw on the high-precision USQCD ensemble in Sec. 4.2.4. $G_A^v(Q^2)$ increases with source-sink separation at low $Q^2$ and it decreases with source-sink separation at larger $Q^2$. On the $m_\pi = 149$ MeV ensemble, which we suspect is affected by thermal contamination at $Q^2 = 0$, the behavior is different: for all $Q^2$, the middle source-sink separation yields lower values of $G_A^v(Q^2)$ than the smallest source-sink separation. This suggests that the axial form factor is affected by the presence of thermal pion states for a range of $Q^2$.

To find the axial radius, we perform dipole fits to $G_A^v(Q^2)$, for $0 \leq Q^2 \leq 0.5$ GeV$^2$. These fits work well, with $\chi^2$/dof $\lesssim 1.5$ even when fitting to the precise data with the shortest source-sink separation. The resulting $(r_A^2)^v$ values are shown in Fig. 5-15. These lie well below the experimental result $[\text{BABAR}]^8$ from quasielastic neutrino scattering ($\nu_\mu n \rightarrow \mu^- p$) on deuterium and from pion electroproduction. Some of the more recent neutrino experiments with heavier target nuclei have yielded larger values of the axial mass ($m_A^2 \equiv \frac{12}{(r_A^2)^v}$), assuming dipole behavior for $G_A^v(Q^2)$ that are compatible with these lattice results, such as MiniBooNE $[\text{AA}^+10]$ ($(r_A^2)^v = 0.26(6) \text{ fm}^2$) and K2K $[\text{G+06}]$ ($(r_A^2)^v = 0.32(6) \text{ fm}^2$).

We extrapolate the product $g_A(r_A^2)^v$ to the physical pion mass using Eq. A.10 which says that to the order in ChPT that we are working at, this product is independent of $m_\pi$. Because this depends on $g_A$, which has significant effects from thermal contamination, we use the same procedure as used for extrapolating $g_A$ and fit to the ensembles with $m_\pi L_t > 7$; the result is shown in Fig. 5-16. All of the fits are of good quality, with $\chi^2$/dof $< 1$. The extrapolated values increase with source-sink separation but are well below the experimental point. There is a significant difference between the summation and GPoF values, indicating that excited states are poorly controlled. Clearly this observable warrants a more-careful study of systematics once $g_A$ is well-understood.

We show the isovector induced pseudoscalar form factor $G_P^v(Q^2)$, computed on the two main ensembles, in Fig. 5-17. Both ensembles show similar behavior, with large excited-state effects at small $Q^2$. These were also very large on the high-precision test ensemble. Having similar behavior on the $m_\pi = 149$ MeV ensemble suggests that the effects caused by thermal pion states might not be as severe as they were for $G_A^v(Q^2)$.

For comparison to experiment, we look to ordinary muon capture on the proton, which is sensitive to $g_P^v \equiv \frac{m_\mu}{2m_N} G_P^v(0.88m_\mu^2)$. Since $G_P^v(Q^2)$ contains a pion pole, we normalize it to its physical value, defining

$$g_P^{\text{norm}} \equiv \frac{m_\mu}{2m_N} \frac{m_\pi^2 + 0.88m_\mu^2}{m_{\pi,\text{phys}}^2 + 0.88m_\mu^2} G_P^v(0.88m_\mu^2), \quad (5.5)$$

where $m_\pi$ and $m_N$ are the masses computed on each lattice ensemble. Extrapolation to $Q^2 = 0.88m_\mu^2$ is done by fitting the lattice $G_P^v(Q^2)$ for $0 < Q^2 \leq 0.5$ GeV$^2$ on
Figure 5-14: Comparison of the isovector axial form factor, computed using different methods, on the $m_\pi = 149$ MeV ensemble and the $32^3 \times 48$, $m_\pi = 254$ MeV ensemble.
each ensemble with a pion-pole plus constant function, as given by ChPT in Eq. A.9. If the location of the pole is fixed using the pion mass determined from the lattice calculation, then the resulting two-parameter fits are somewhat poor when fitting to more-precise data. For instance, fitting the middle source-sink separation on the $m_\pi = 149$ MeV ensemble yields $\chi^2$/dof = 41/19. Including the pole location as a fit parameter yields a better fit with $\chi^2$/dof = 22/18, but the pole mass is 227(18) MeV, well above the pion mass on this ensemble; this behavior was previously observed in Ref. BEE+10. Fitting to the less-precise data on the $m_\pi = 149$ MeV ensemble (i.e. using summation, GPoF, or the largest source-sink separation), while setting the pole position to the calculated pion mass, gives reasonable values of $\chi^2$ between 20 and 28. Despite these issues, we proceed by fitting with the pole mass set to the calculated pion mass, knowing that a fitted pole mass would generally be larger, which leads to smaller values of $g_P^{\text{norm}}$.

The resulting values of $g_P^{\text{norm}}$ are shown in Fig. 5-18. The high-precision study done on the USQCD ensemble shows that excited-state effects are quite large, and we should not consider them as under control. The data broadly increase with $m_\pi$, and the results on the smaller-volume ensembles have large statistical errors; as was the case with $F_2(Q^2)$, the extrapolation to $Q^2 = 0.88m_\mu^2$ on these ensembles is more difficult. We use the two-parameter ChPT formula, Eq. A.11, to extrapolate to the physical pion mass as shown in Fig. 5-19. The extrapolated values are well below the experimental measurement. Better fits to $G_P^v(Q^2)$ would generally move the data away.
Figure 5-16: Isovector axial radius multiplied by the axial charge, \( g_A(r_A^2) v \), from dipole fits to \( G_A^v(Q^2) \) computed using the summation method, and chiral extrapolation to the physical pion mass. Points in red are included in the fit. On the left, the extrapolated values computed using other methods are also shown; see the legend of Fig. 5-15.
Figure 5-17: Comparison of the isovector induced pseudoscalar form factor, computed using different methods, on the $m_\pi = 149$ MeV ensemble and the $32^3 \times 48, m_\pi = 254$ MeV ensemble.
Figure 5-18: Induced pseudoscalar coupling $g_p^{\text{norm}}$ from fits on the BMW and USQCD ensembles (see text); see the caption of Fig. 5-4. The value from the MuCap experiment $^{A+13}$ is also shown.

from the experimental point, but it seems likely that improved control over excited states would move the data toward the experimental point.

### 5.3 Isovector quark momentum fraction

The isovector quark momentum fraction, $\langle x \rangle_{u-d} \equiv A_{20}^v(0)$, is shown in Fig. 5-20. This observable shows clear signs of strong excited-state effects, as was seen in the high-precision study. Although using the summation or GPoF method causes the calculation on the $m_\pi = 149$ MeV ensemble to agree with phenomenology, more work is needed to achieve good control over excited-state systematics. Extrapolation to the physical pion mass is shown in Fig. 5-21; this also produces agreement with the phenomenological result.

### 5.4 Neutron beta decay couplings

The scalar charge $g_S$ is shown in Fig. 5-22; the results suffer from much larger statistical errors than the axial charge. Relative to these large statistical errors, there do not appear to be significant effects from excited states, finite volumes, or discretization. Even on the high-precision ensemble, excited-state effects appear to be absent from the middle source-sink separation. Therefore, we use the ratio-plateau method with
Figure 5-19: Induced pseudoscalar coupling $g_{\text{P}}^{\text{norm}}$, from fits to $G_{\text{P}}(Q^2)$ computed using the summation method, and chiral extrapolation to the physical pion mass. Points in red are included in the fit. On the left, the extrapolated values computed using other methods are also shown; see the legend of Fig. 5-18.
Figure 5-20: Isovector average quark momentum fraction on the BMW and USQCD ensembles; see the caption of Fig. 5-4. The normalization used on the USQCD ensemble is arbitrary, as we have not computed a renormalization factor. The CTEQ6 [PSH+02] phenomenological value is also shown.
Figure 5-21: Isovector quark momentum fraction computed using the summation method, and chiral extrapolation to the physical pion mass. Points in red are included in the fit. On the left, the extrapolated values computed using other methods are also shown; see the legend of Fig. 5-20.
Due to poor constraints from phenomenology, we have three free parameters in our extrapolation formula, Eq. A.14. Therefore, we choose to fit to the full range of pion masses, selecting the larger volumes at each pion mass; this is shown in Fig. 5-23. The fits are of good quality with $\chi^2$/dof $< 1$, and the extrapolated values are consistent with the absence of excited-state effects. We estimate finite-volume effects by comparing the $24^3 \times 48$ and $24^3 \times 48$ ensembles at $m_\pi \approx 250$ MeV, assuming that the effects scale as $e^{-m_\pi L_s}$. We similarly estimate thermal effects by comparing ensembles at $m_\pi \approx 250$ and 350 MeV and assuming that the effects scale as $e^{-m_\pi L_t}$.

On the $m_\pi = 149$ MeV ensemble, these scaling assumptions imply that $g_S$ is shifted by $-0.11(17)$ due to finite $L_s$ and by $0.15(19)$ due to finite $L_t$. Since this ensemble has the largest effect on the extrapolation, we use the central value of the estimated effect of finite spatial and temporal extents on that ensemble in order to get the final prediction:

$$g_S^{\text{MS}(2 \text{ GeV})} = 1.04 \pm 0.27 \text{ (stat)} \pm 0.11 \text{ (} L_s \text{)} \pm 0.15 \text{ (} L_t \text{)}.$$

(5.6)

Based on the high-precision test ensemble, we conclude that excited-state systematics are somewhat smaller than the quoted errors. The dominant error is statistical, and it can be improved either with higher-statistics calculations near the physical pion mass, or with better phenomenological input to chiral perturbation theory so that ensembles at larger-than-physical pion masses are better at constraining the extrapolation. An alternative determination of $g_S$ can be had via the Feynman-Hellmann theorem, which...
Figure 5-23: Scalar charge computed using the ratio-plateau method with the middle source-sink separation, and chiral extrapolation to the physical pion mass. Points in red are included in the fit. On the left, the extrapolated values computed using other methods are also shown; see the legend of Fig. 5-22.
implies, to leading order,

\[ g_s = \frac{(m_p - m_n)_{\text{QCD}}}{m_u - m_d}. \]  

Combining the recent calculation [BDF+13] by BMW of octet baryon mass isospin splittings in lattice QCD+QED with their earlier calculation [DFH+11] of light quark masses using lattice QCD (which yielded \(m_u + m_d\)) and phenomenology (to find \(m_u, m_d\) individually) yields \(g_s = 0.86(11)\), in good agreement with our result.

We show the tensor charge \(g_T\) in Fig. 5-24 As with the scalar charge, it appears that excited-state effects are not very large, but this is not nearly as noisy. We again select the middle source-sink separation data as our main results; their extrapolation using Eq. A.16 is shown in Fig. 5-25. The best-fit parameters have \(\mu^2 = 0\), which removes the chiral log, but the fits are good with \(\chi^2/\text{dof} < 1.1\) since the dependence on \(m_\pi\) is very mild. We estimate effects from finite \(L_s\) and \(L_t\) in the same way as for the scalar charge; the scaling assumptions imply a shift by \(0.020(25)\) due to \(L_s\) and by \(-0.037(25)\) due to \(L_t\). Although high-precision calculations on the USQCD ensemble suggest that excited-state effects are quite small, we nevertheless estimate their size from the difference between our main extrapolated value and that computed using the shortest source-sink separation. Together, these give the final prediction:

\[ g_T^{\overline{\text{MS}}}(2\ \text{GeV}) = 1.036 \pm 0.010 \text{ (stat)} \pm 0.020 \text{ (}L_s\text{)} \pm 0.037 \text{ (}L_t\text{)} \pm 0.012 \text{ (exc. states).} \]  

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Figure 5-25: Tensor charge computed using the ratio-plateau method with the middle source-sink separation, and chiral extrapolation to the physical pion mass. Points in red are included in the fit. On the left, the extrapolated values computed using other methods are also shown; see the legend of Fig. 5-24.

If these errors are added in quadrature, the combined error is less than 5%. The main unestimated source of error is discretization, but comparison with our calculations done using fine (\( a = 0.084 \text{ fm} \)) domain-wall ensembles in Ref. [GNP+12] suggests that discretization effects are not more than a few percent. Other than the need to obtain control over the continuum limit, the dominant uncertainty is from thermal effects; reducing this would be a side-benefit to calculations done for understanding the influence of thermal states on the axial charge. However, the error is already well below the 10–20% level that Ref. [BCC+12] stated was sufficient for upcoming neutron beta-decay experiments.

### 5.5 Isoscalar observables

We also examine a few isoscalar observables. Because we have not computed the required quark-connected contractions, these suffer from an additional uncontrolled systematic error. We will not perform an extrapolation to the physical pion mass; rather, this examination will serve to provide qualitative information about the relevance of different sources of systematic error and the dependence on pion mass. In the absence of signs of other systematic errors, comparing the \( m_\pi = 149 \text{ MeV} \) ensemble and experiment gives an indication of the possible size of disconnected contributions.

The isoscalar Dirac radius, determined from dipole fits to \( F_1^s(Q^2) \), is shown in
Figure 5-26: Isoscalar Dirac radius from dipole fits on the BMW and USQCD ensembles; see the caption of Fig. 5-4. We show two experimental values, where $(r_E^2)^p$ is taken from either the CODATA 2010 result [MTN12] used by the PDG [B+12] or the measurement from spectroscopy of muonic hydrogen [ANS+13]. Both points use the PDG value for $(r_E^2)^n$. 
Figure 5-27: Quark spin contribution to the nucleon angular momentum, $\frac{1}{2}\Delta \Sigma_{u+d}$, on the BMW and USQCD ensembles; see the caption of Fig. 5-4. The experimental point is from HERMES [A+07].

Fig. 5-26. As with the isovector Dirac radius, control over excited-state effects is important, particularly at the lightest pion masses. The same set of heavy baryon ChPT expressions that we used for the isovector Dirac radius say that the isoscalar Dirac radius is independent of $m_\pi$. Since we see that $(r_1^2)^{\pi}$ rises toward the experimental values as the pion mass decreases, it is clear that these ChPT expressions are not a good description of our data.

Figure 5-27 shows the total $u+d$ quark spin contribution to the nucleon angular momentum, $\frac{1}{2}\Delta \Sigma_{u+d} \equiv \frac{1}{2}G_A^{u+d}(0)$. The high-precision ensemble indicates that excited-state effects are small, and the other ensembles don’t have a consistent dependence on source-sink separation. Because the isovector equivalent of this quantity, $g_A$, had significant thermal effects, it is interesting to note that the same behavior is not apparent here. Comparing the ensembles with small $m_\pi L_t$ against the others does not reveal the same dramatic behavior that we saw for $g_A$. The calculations done on the $m_\pi = 149$ MeV ensemble agree with the experimental result; this suggests that disconnected contributions are not large.

In Fig. 5-28 we show the isoscalar equivalent of the tensor charge, which is the first moment of transversity $\langle 1 \rangle_{\delta u+\delta d}$. As with the isovector quantity, this appears fairly well behaved, with small excited-state effects and little dependence on $m_\pi$. With an unknown error from the omission of disconnected diagrams, these results support a prediction of roughly 0.6, which will be tested at Jefferson Lab.
5.6 Conclusions

The two major advances in these calculations are the use of a near-physical pion mass and the reduction of excited-state effects; this combination produced agreement with experiment for the nucleon isovector Dirac and Pauli radii, anomalous magnetic moment, and quark average momentum fraction. The importance of excited-state systematics was clearly demonstrated, and more work is still needed to obtain better control over them. Although reduced statistical errors and somewhat better control over the other systematics (discretization and finite $L_s$ and $L_t$) are also needed, these are promising results that suggest lattice QCD calculations may be able to contribute to a resolution of the proton radius problem.

For the axial charge, distinctive behavior for ensembles with small $m_\pi L_t$ indicates that thermal pion states may be affecting the result. Restricting the analysis to ensembles with larger values of $m_\pi L_t$ leads to the same conclusion as Ref. [CDMvH+12], which is that agreement with experiment can only be achieved with good control over excited states. We also find that excited states are important for the axial radius $(r_A^2)^v$ and the induced pseudoscalar coupling $g_P^{\text{norm}}$, although our extrapolated results lie well below experiment. Performing calculations on an ensemble with a near-physical pion mass and a large time extent would help to resolve the issue.

Finally, Eqs. 5.6 and 5.8 contain our predictions for the scalar and tensor charge. The latter will be tested in experiments at Jefferson Lab, and both of them should provide useful inputs to beta-decay experiments.
Appendix A

Chiral perturbation theory

We will largely use the same methods and phenomenological inputs for chiral perturbation theory as Refs. [GEK+12a, BEE+10]. In particular, we use the following values in the chiral limit: the pion decay constant,

\[ F_\pi = 86.2 \text{ MeV}, \]  

(A.1)

the delta-nucleon mass splitting,

\[ \Delta = 293 \text{ MeV}, \]  

(A.2)

and the nucleon axial charge,

\[ g_A = 1.26. \]  

(A.3)

A.1 Isovector vector form factors

The nucleon isovector Dirac and Pauli form factors are given in heavy baryon ChPT including the delta baryon, to order \( \epsilon^3 \) in the small-scale expansion (\( \epsilon \in \{ p, m_\pi, \Delta \} \)) in Ref. [BFHM98]. This gives an expression for the Dirac radius [SBL+10],

\[
(r_1^v)^2 = -\frac{1}{(4\pi F_\pi)^2} \left[ 1 + 7g_A^2 + (2 + 10g_A^2) \log \left( \frac{m_\pi}{\lambda} \right) \right] - \frac{12B_{10}^v(\lambda)}{(4\pi F_\pi)^2} \\
+ \frac{c_A^2}{54\pi^2 F_\pi^2} \left[ 26 + 30 \log \left( \frac{m_\pi}{\lambda} \right) + 30 \frac{\Delta}{\sqrt{\Delta^2 - m_\pi^2}} \log \left( \frac{\Delta}{m_\pi} + \sqrt{\frac{\Delta^2}{m_\pi^2} - 1} \right) \right],
\]  

(A.4)

where \( c_A \) is the leading-order pion-nucleon-delta coupling in the chiral limit, which we set to 1.5 [SBL+10], and \( B_{10}^v(\lambda) \) is a counterterm and the single free parameter.

For the anomalous magnetic moment, we include the modification from Ref.
The nucleon axial charge is given in heavy baryon ChPT with delta degrees of freedom. To order \( \mathcal{O}(\kappa^2) \), the combination \( \kappa^v(r_2^v)^2 \) is more natural in ChPT than the Pauli radius alone; we include the \( O(m_0^4) \) “core” contribution from Ref. [GHH+05] in the expression for it:

\[
\kappa^v(r_2^v)^2 = \frac{g_A^2 m_N}{8\pi F_\pi^2 m_\pi} + \frac{c_A^2 m_N}{9\pi^2 F_\pi^2 \Delta^2 - m_\pi^2} \log \left( \frac{\Delta}{m_\pi} + \sqrt{\frac{\Delta^2}{m_\pi^2} - 1} \right) + 24m_N \mathcal{C},
\]

(A.6)

where \( \mathcal{C} \) is the single free parameter.

### A.2 Isovector axial form factors

The nucleon axial charge is given in heavy baryon ChPT with delta degrees of freedom to order \( \epsilon^3 \) in the small-scale expansion in Ref. [HPW03]:

\[
g_A(m_\pi) = g_A - \frac{g_A^3 m_\pi^2}{16\pi^2 F_\pi^2} + 4m_\pi^2 \left[ C(\lambda) + \frac{c_A^2}{4\pi^2 F_\pi^2} \left( \frac{155}{972} g_1 - \frac{17}{36} g_A \right) + \gamma \log \frac{m_\pi}{\lambda} \right]
\]

\[
+ \frac{4c_A^2 g_A}{27\pi^2 F_\pi^2 \Delta} m_\pi^3 + \frac{8c_A^2 g_A m_N^2}{27\pi^2 F_\pi^2} \sqrt{1 - \frac{m_\pi^2}{\Delta^2}} \log \left( \frac{\Delta}{m_\pi} + \sqrt{\frac{\Delta^2}{m_\pi^2} - 1} \right)
\]

\[
+ \frac{c_A^2 \Delta^2}{81\pi^2 F_\pi^2} \left( 25g_1 - 57g_A \right) \left[ \log \frac{2\Delta}{m_\pi} - \sqrt{1 - \frac{m_\pi^2}{\Delta^2}} \log \left( \frac{\Delta}{m_\pi} + \sqrt{\frac{\Delta^2}{m_\pi^2} - 1} \right) \right],
\]

(A.7)

where \( g_1 \) controls the delta axial charge and we set it to 2.5 [BEE+10], and we keep \( g_A \) and the counterterm \( C(\lambda) \) as free parameters.

To the same order, dependence on \( Q^2 \) of the isovector axial form factors is given...
in Ref. [BFHM98]:

\[ G_A^{v}(Q^2, m_\pi) = g_A(m_\pi) - \frac{Q^2}{(4\pi F_\pi)^2} \bar{B}_3 \]  

(A.8)

\[ G_P^{v}(Q^2, m_\pi) = \frac{4m_N^2}{m_\pi^2 + Q^2} \left( g_A(m_\pi) - \frac{2m_\pi^2 \bar{B}_2}{(4\pi F_\pi)^2} \right) - \bar{B}_3 \frac{4m_N^2}{(4\pi F_\pi)^2} . \]  

(A.9)

In particular, this means that the product,

\[ g_A(r_A^2)^v \equiv -6 \left. \frac{dG_A^v}{dQ^2} \right|_{Q^2=0} = \frac{6 \bar{B}_3}{(4\pi F_\pi)^2}, \]  

(A.10)

has one parameter (the counterterm \( \bar{B}_3 \)) and is independent of \( m_\pi \). We also make use of the quantity (with \( Q^2 = 0.88m_\mu^2 \))

\[ g_P^{\text{norm}}(m_\pi) \equiv \frac{m_\mu(m_\pi^2 + Q_\pi^2)}{2m_N(m_\pi^2_{\text{phys}} + Q_\pi^2)} G_P^{v}(Q_\pi^2) = \frac{2m_\mu m_N}{m_\pi^2_{\text{phys}} + Q_\pi^2} \left( g_A(m_\pi) - \frac{m_\pi^2}{(4\pi F_\pi)^2} \left( 2\bar{B}_2 + \bar{B}_3 \right) - \frac{Q_\pi^2}{(4\pi F_\pi)^2} \bar{B}_3 \right) , \]  

(A.11)

which has the same dependence on \( m_\pi \) as \( g_A(m_\pi) \), except for: an overall scaling factor; the replacement of the counterterm \( C(\lambda) \) with a linear combination of \( C(\lambda) \), \( \bar{B}_2 \), and \( \bar{B}_3 \); and an overall shift proportional to \( \bar{B}_3 \). For fitting to \( g_P^{\text{norm}}(m_\pi) \), we additionally fix \( g_A \) to its phenomenological value, leaving two free parameters, which are counterterms.

### A.3 Isovector generalized form factors

Form factors of the isovector quark energy-momentum operator are given to \( O(p^2) \) in covariant baryon ChPT in Ref. [DGH08]. In particular, the quark momentum fraction
is given by

\[
\langle x \rangle_{u-d} \equiv A_{20}^v(0)
\]

\[
= a_{20}^v + \frac{a_{20}^v m_\pi^2}{4\pi F_\pi^2} \left[ (-3g_A^2 + 1) \log \frac{m_\pi^2}{\lambda^2} - 2g_A^2 + g_A^2 \frac{m_\pi^2}{m_{N,0}^2} \left( 1 + 3 \log \frac{m_\pi^2}{m_{N,0}^2} \right) 
\right.
\]

\[
- \frac{g_A^2 m_\pi^4}{2 m_{N,0}^4} + \frac{g_A^2 m_{N,0}}{\sqrt{m_{N,0}^2 - m_\pi^2}} \left( 14 - 8 \frac{m_\pi^2}{m_{N,0}^2} + \frac{m_\pi^4}{m_{N,0}^4} \right) \arccos \frac{m_\pi}{2m_{N,0}} \left] + \frac{\Delta a_{20}^v g_A m_\pi^2}{3(4\pi F_\pi)^2} \left[ 2 \frac{m_\pi^2}{m_{N,0}^2} \left( 1 + 3 \log \frac{m_\pi^2}{m_{N,0}^2} \right) - \frac{m_\pi^4}{m_{N,0}^4} \log \frac{m_\pi^2}{m_{N,0}^2} 
\right.
\]

\[
+ \frac{2m_\pi(4m_{N,0}^2 - m_\pi^2)^{3/2}}{m_{N,0}^4} \arccos \frac{m_\pi^2}{2m_{N,0}} \left] + 4c_8^\tau(\lambda) \frac{m_\pi^2}{m_{N,0}^2}, \right.
\]

\[\text{(A.12)}\]

where \(a_{20}^v\), \(\Delta a_{20}^v\), and \(m_{N,0}\) are the isovector momentum fraction \(\langle x \rangle_{u-d}\), isovector polarized momentum fraction \(\langle x \rangle_{\Delta u-\Delta d}\), and nucleon mass, respectively, in the chiral limit. We fit by fixing the phenomenological values \(m_{N,0} = 873\) MeV and \(\Delta a_{20}^v = 0.165\), keeping \(a_{20}^v\) and the counterterm \(c_8^\tau(\lambda)\) as the two free parameters.

### A.4 Scalar charge

For chiral extrapolation of the scalar charge, we make use of the Feynman-Hellmann theorem to obtain

\[
g_S \equiv \langle p|\bar{u}u - \bar{d}d|p\rangle = \left( \frac{\partial}{\partial m_u} - \frac{\partial}{\partial m_d} \right) M_p. \tag{A.13}\]

Strong isospin splitting of nucleon masses has been computed in \(SU(2)\) heavy baryon ChPT, with explicit \(\Delta\) degrees of freedom, to next-to-next-to-leading-order, i.e. to \(O(m_q^3)\) \cite{TWL06}. This leads to the expression

\[
g_S(m_\pi^2) = 2\alpha_M
\]

\[
- \frac{1}{2(4\pi F_\pi)^2} \left\{ m_\pi^2 \left[ 8(g_A^2 \alpha_M + g_{\Delta N}^2 (\alpha_M + \frac{5}{9} \gamma_M)) - (b_1^M + b_6^M) \frac{\pi(\sqrt{2}F_\pi)^3}{\lambda} \right] 
\right.
\]

\[
+ m_\pi^2 \log \left( \frac{m_\pi^2}{\mu^2} \right) 2\alpha_M (6g_A^2 + 1) + \mathcal{J}(m_\pi, \Delta, \mu) 8g_{\Delta N}^2 (\alpha_M + \frac{5}{9} \gamma_M) \right\}, \tag{A.14}\]
where
\[
\mathcal{F}(m, \Delta, \mu) = (m^2 - 2\Delta^2) \log \frac{m^2}{\mu^2} + 2\Delta \sqrt{\Delta^2 - m^2} \log \left( \frac{\Delta - \sqrt{\Delta^2 - m^2 + i\epsilon}}{\Delta + \sqrt{\Delta^2 - m^2 + i\epsilon}} \right) + 2\Delta^2 \log \frac{4\Delta^2}{\mu^2}.
\] (A.15)

Fixing \(g_A, F_\pi,\) and \(\Delta\) as usual leaves 3 independent parameters to which we fit our \(g_S(m_\pi^2)\) data: \(\alpha_M\) and \(\gamma_M\), which control the leading-order nucleon and delta strong isospin splitting, respectively, and the combination of low-energy constants \(b_1^M + b_6^M\).

### A.5 Tensor charge

Chiral extrapolation formulas for the tensor charge are given in [DMT02]. Full formulas including \(\Delta\) loops are given via a number of integrals, and then it is shown that these are approximated well by an expression that includes only the leading non-analytic term. Finally, including terms that connect to the heavy quark limit yields the expression:

\[
g_T(m_\pi^2) = \delta a \left( 1 + \delta c_{\text{LNA}} m_\pi^2 \log \frac{m_\pi^2}{m_\pi^2 + \mu^2} \right) + \delta b \frac{m_\pi^2}{m_\pi^2 + m_b^2},
\] (A.16)

where from the heavy quark limit

\[
\delta b = \frac{5}{3} - \delta a (1 - \mu^2 \delta c_{\text{LNA}}),
\] (A.17)

and the coefficient of the log term is

\[
\delta c_{\text{LNA}} = \frac{-1}{2(4\pi F_\pi)^2} \left[ \left( 2 - \frac{4 g_{\pi N}^2}{9 g_{\pi NN}^2} \right) g_A^2 + \frac{1}{2} \right].
\] (A.18)

We fix \(m_b = 5\) GeV and \(\frac{g_{\pi N A}}{g_{\pi NN}} = 1.85\) as in [DMT02] to obtain a fit with 2 independent parameters.
A. Airapetian et al., *Precise determination of the spin structure function \( g_1 \) of the proton, deuteron and neutron*, Phys. Rev. D 75, 012007 (2007), arXiv:hep-ex/0609039.


C. Alexandrou, M. Constantinou, S. Dinter, V. Drach, K. Jansen, et al., *Nucleon form factors and moments of generalized parton distributions using \( N_f = 2 + 1 + 1 \) twisted mass fermions*, arXiv:1303.5979 [hep-lat].


