Derivatives of matrix element from Lattice QCD

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Momentum-space derivatives of matrix elements can be related to their coordinate-space moments through the Fourier transform. We derive these expressions as a function of momentum transfer Q^2 for asymptotic in/out states consisting of a single hadron. We calculate corrections to the finite volume moments by studying the spatial dependence of the lattice correlation functions. This method permits the computation of not only the values of matrix elements at momenta accessible on the lattice, but also the momentum-space derivatives, providing a priori information about the Q^2 dependence of form factors. As a specific application we use the method, at a single lattice spacing and with unphysically heavy quarks, to directly obtain the slope of the isovector form factor at various Q^2, whence the isovector charge radius. The method has potential application in the calculation of any hadronic matrix element with momentum transfer, including those relevant to hadronic weak decays.

I. INTRODUCTION

Answers to some of the deepest mysteries of nature may be uncovered through fundamentally understanding how protons and neutrons, the basic building blocks of our world, interact with the universe. The lattice QCD community has contributed to our understanding of the strength of these interactions by direct calculations of form factors. In this work, we propose a method to directly calculate the slope of these form factors, which shed light on new ways to test our current understanding of the Standard Model.

A. On the radius of the proton

The charged leptons are fundamental (point-like) particles in the Standard Model of particle physics, with identical coupling strengths to the electroweak currents, and only differ in mass between the three generations. This Standard Model paradigm, known as *lepton universality*, is however, in tension with recent experimental observations of the proton charge radius [1]. In particular, measurement from muonic Hydrogen [2] resulted in a 4% smaller proton radius when compared to the CODATA average from 24 transition frequency measurements of atomic Hydrogen [3], in tension at 4 standard deviations. This discrepancy hints at the possibility that the electron and muon may differ fundamentally in ways unaccounted for by the Standard Model. Recently, evidence of possible resolution to the proton radius puzzle was provided by an updated measurement of the 2S-4P transition frequency [4] that is consistent with the muonic Hydrogen measurement. However, a recent update on the 1S-3S transition frequency [5] continues to re-enforce the discrepancy between atomic and muonic experiments. Additionally, recent electron scattering results continue to exhibit the long standing discrepancy with muonic Hydrogen [6]. Due to the vast number of transition frequencies from Lamb shift measurements, and tension from the electron scattering result, resolution to the charge radius puzzle may still require considerable additional effort from experimentalists. Furthermore, the ratio of semi-leptonic $B \to D^{(*)}\ell\bar{\nu}$ decays to the electron and tau final states is also observed to be in tension with the Standard Model prediction at 4 standard deviations [7], lending evidence that the discrepancy seen in the proton radius may in fact be a result of new physics.

While the measurement of the proton radius is very challenging, its definition is straightforward from a theory stand point. Specifically, the charge radius of the proton is defined as the Q^2 (momentum-squared) derivative of the vector form factor $F_V(Q^2)$ evaluated at zero-momentum transfer, and may be directly calculated from QCD using lattice methods. Current LQCD determinations of the radius however, leave much to be desired, because the derivative is extracted from modeling the Q^2 dependence of F_V from calculations at discrete values of momentum accessible in a finite volume. Such calculations are susceptible to two major problems: first, the model dependence introduces uncontrolled systematic errors, and additionally, the smallest non-zero momentum is too large to perform a controlled extrapolation of the slope at zero-momentum since accessing small momentum in finite volumes requires very large lattices that are prohibitively expensive.

B. On the origin of matter

One of the outstanding mysteries of our universe lies in quest to understand the origin of matter, or more specifically the origin of the matter-antimatter asymmetry that we observe today. There is tantalizing evidence for possible sources of *leptogenesis* recently revealed at the *Tokai-2-Kamioka* (T2K) long-baseline neutrino experiment [8], where CP conservation in the neutrino sector is excluded at 90% confidence. Future long-baseline neutrino experiments including the *Deep Underground Neutrino Experiment* (DUNE), and the detector upgrade to Hyper-Kamiokande (T2HK) aims to provide more precise neutrino oscillation measurements in order to further resolve the neutrino CP-violating phase. Additionally, cost-effective projects such as *CHerenkov detectors In mine PitS* (CHIPS) [9], a water Cherenkov detector designed to be approximately 5 times larger than Super-Kamiokande, is planned with the intention to ultimately run off the DUNE beamline, providing a cost-efficient way to improve knowledge on neutrino parameters including the CP violating phase.

In order to fully benefit from the advances of next generation neutrino experiments, the theoretical description of neutrino scattering must also be made more precise through improving the current determination of the nucleon axial form factor $F_A(Q^2)$. The axial form factor parameterizes the strength in which the weak current couples to the nucleon, and consequently governs the neutrino scattering cross-section off nuclear targets in the regime of quasi-elastic scattering. There is currently a 1–2% uncertainty on the determination of the cross-section [10] that is dominated by the hadronic uncertainty on the axial form factor at small momentum transfer up to approximately 1 GeV [11]. Similar to the determination of the charge radius, the shape of the form factor is often derived from the model dependent dipole ansatz. Recent progress in lattice QCD has demonstrated control at the percent-level over the axial form factor at zero-momentum transfer [12]. The method introduced in this paper is extensible to calculations of the slope at non-zero momentum transfer and paves a way for controlling the full momentum dependence of the form factor at the same level of precision.

C. Overview

Need to write some outline paragraph. Highlight some main results and advantages of this method. Possible content: Main result: Introduce method for direct slope calculation. Main improvements: 1) Model independent 2) Does not require small momentum data, direct zero momentum evaluation.

II. MOMENTS OF CORRELATION FUNCTIONS

This part is only slightly reworded from the proceedings. I am pointing this out in case any one thinks it's a problem. Position-space moment methods was first introduced to calculate the slope of the Isgur-Wise function $\xi(w)$ at zero-recoil, in order to interpret experimental results near zero-recoil for $B \to D$ semi-leptonic decays [13], and later adapted to calculate the slope of the energy-momentum tensor form factor, yielding the angular momentum contribution to the spin of the nucleon [14, 15]. Recently, there is revitalized interest in applying moment methods to calculate the hadronic vacuum polarization [16, 17], and efforts to directly determine the anomalous magnetic moment of the nucleon and radii in nuclear physics [18]. In parallel, momentum-space derivative methods are also being explored to access similar nucleon structure calculations such as the anomalous magnetic moment and various nucleon radii [19, 20]. In this work, we present a coordinate-space method that directly calculates the slope of single particle form factors with respect to the squared momentum-transfer at any lattice accessible momenta.

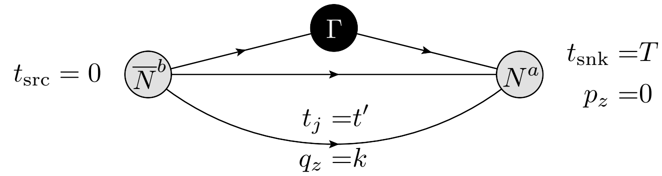

FIG. 1. Kinematics of the three-point correlator with baryon initial and final states. We work in the rest frame of the final hadron. The diagram for semi-leptonic decays of mesons involves only one spectator quark, but involves the same kinematics. Change a and b to say src and snk.

A. Formalism

Some more self-plagiarism.

1. *Three-point correlation function*

Given a three-point correlation function with the initial state at rest, and current insertion with three-momentum k, where k points in the z-direction without loss of generality, as shown in Fig. 1, the three-momentum-projected three-point has the general form,

$$C^{3\rm pt}(t,t') = \sum_{\vec{x},\vec{x}'} \left\langle N^{\rm snk}_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^{\rm src}_{0,\vec{0}} \right\rangle e^{-ikx'_z}, \tag{1}$$

translational invariance allows us to shift the source to the origin $\vec{x}_{\rm src} = 0$ and the sink to $\vec{x} \equiv \vec{x}_{\rm snk} - \vec{x}_{\rm src}$. Since the sink has zero three-momentum, the only momentum dependence left is at the current insertion. The operators $N^{\rm src}$ and $N^{\rm snk}$ are the source and sink interpolation operators respectively, allowing for different choices of the nucleon interpolating operator [21, 22] and operator smearing profiles. The operator Γ is a generic current insertion at position $\vec{x}' \equiv \vec{x}_J - \vec{x}_{\rm src}$.

The derivative of the three-point correlator with respect to k^2 follows,

$$C'_{3\rm pt}(t,t') = \sum_{\vec{x},\vec{x}'} \frac{-x'_z}{2k} \sin\left(kx'_z\right) \left\langle N^{\rm snk}_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^{\rm src}_{0,\vec{0}} \right\rangle, \tag{2}$$

where in Eq. (2), the cosine component vanishes due to symmetry. In the limit of zero momentum, the $k^2 \to 0$ limit of the integrand is given by L'Hôpital's rule,

$$\lim_{k^2\to 0} C'_{3\mathrm{pt}}(t,t') = \sum_{\vec{x},\vec{x}'} \frac{-x_z'^2}{2} \left\langle N^{\mathrm{snk}}_{t,\vec{x}} \Gamma_{t',\vec{x}'} \overline{N}^{\mathrm{src}}_{0,\vec{0}} \right\rangle . \tag{3}$$

While it is tempting to think of Eq. (3) as having an $x_z'^2$ moment, it is clear from Eq. (2), that a single derivative contributes only a single factor of x'_z. The second factor of x'_z only appears in the $k^2 \to 0$ limit and should not be thought as a position-space moment resulting from a momentum-space derivative.

2. Two-point correlation function

Analogously, given a two-point correlator with three-momentum k in the z-direction,

$$C_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \left\langle N^{\mathrm{snk}}_{t,\vec{x}} \overline{N}^{\mathrm{src}}_{0,\vec{0}} \right\rangle e^{-ikx_z}, \tag{4}$$

the derivative of the two-point correlator with respect to k^2 follows,

$$C'_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \frac{-x_z}{2k} \sin(kx_z) \left\langle N^{\mathrm{snk}}_{t,\vec{x}} \overline{N}^{\mathrm{src}}_{0,\vec{0}} \right\rangle . \tag{5}$$

Analogous to the moment of the three-point correlator, the cosine contribution vanishes due to symmetry. Consequently, in the zero-momentum limit,

$$\lim_{k^2\to 0} C'_{2\mathrm{pt}}(t) = \sum_{\vec{x}} \frac{-x_z^2}{2} \left\langle N^{b}_{t,\vec{x}} \overline{N}^{b}_{0,\vec{0}} \right\rangle . \tag{6}$$

The construction of the moment of the two-point correlator is similar to the moment of the three-point correlator with the exception that the moment now depends on the final state position x_z instead of the current insertion position x'_z. In both cases, the spatial dependence for all momenta are even, resulting in a non-vanishing correlator under the Fourier transform, explicitly circumventing the concern raised in Ref [23]. Given prior computational investment in generating the propagators and sequential propagators, the generation of the moments of correlators only differ during the Fourier transform, and therefore require negligible additional computing time to construct.

B. Interpretation

1. Three-point correlation function

In the rest frame of the final state hadron, the spectral decomposition of the three-point correlation function in Eq. (1) is

$$C_{3\mathrm{pt}}(t,t') = \sum_{n,m} \frac{Z^{\dagger\mathrm{snk}}_m(0)\Gamma_{mn}(k^2) Z^{\mathrm{src}}_n(k^2)}{4E_m(0)E_n(k^2)} \times e^{-E_m(0)(t-t')} e^{-E_n(k^2)t'} . \tag{7}$$

The time dependence involves the source-sink separation $t \equiv t^{\mathrm{snk}} - t^{\mathrm{src}}$ and the insertion-sink separation $t' \equiv t^{\mathrm{ins}} - t^{\mathrm{src}}$. The parameters $E_n(k^2)$ infer the n-th state energy of the hadron with momentum k^2, $\Gamma_{mn}(k^2)$ infers the $n \to m$-th state matrix element, and $Z^{\mathrm{src(snk)}}_{n(m)}$ infers the overlap factor at the source and sink, which in general is different and depends on the interpolating operator and smearing profile used. On the lattice, the path integral is performed under a Wick rotation, yielding the exponential time dependence. At large time separations, the ground state signal exponentially dominates the correlation function.

Taking the k^2 derivative of Eq. (7) yields the spectral decomposition of the correlator generated by Eqs. (2, 3),

$$C'_{3\mathrm{pt}}(t,t') = \sum_{m,n} C^{mn}_{3\mathrm{pt}}(t,t') \left[\frac{\Gamma'_{mn}(k^2)}{\Gamma_{mn}(k^2)} + \frac{Z'^{\mathrm{src}}_n(k^2)}{Z^{\mathrm{src}}_n(k^2)} - \frac{1}{2E_n^2(k^2)} - \frac{t'}{2E_n(k^2)} \right], \tag{8}$$

where $C^{mn}_{3\mathrm{pt}}$ is the $n \to m$-th state contribution of Eq. (7) and Γ' is the k^2 derivative of the matrix element Γ. Extracting Γ' is the main goal of this paper. An additional consequence is the dependence on Z'^{src}, the k^2 derivative of the source overlap factor, which can be analogously extracted from the derivative of the two-point correlator. Here we note that in the rest-frame of the final hadron, only Z'^{src} survives, while any dependence on Z'^{snk} explicitly vanishes, where the source and sink operators here apply to the three-point correlation function, and in general may be different from the operators used in the two-point correlator in the following discussion.

2. Two-point correlation function

The spectral decomposition of the two-point correlation function constructed from Eq. (4) is,

$$C_{2\mathrm{pt}}(t) = \sum_{m} \frac{Z^{\dagger\mathrm{snk}}_m(k^2) Z^{\mathrm{src}}_m(k^2)}{2E_m(k^2)} e^{-E_m(k^2)t} \tag{9}$$

where on a given lattice, $t \equiv t^{\mathrm{snk}} - t^{\mathrm{src}}$ is the same source-sink separation t in Eqs. (7, 8). While in general, the source and sink operators may be different from the three-point correlation function, at least one of the operators has to be the same as the three-point source operator in order to disentangle Γ' from Z'^{src} from Eq. (8).

Taking the k^2 derivative of Eq. (9) yields,

$$C'_{2\mathrm{pt}}(t) = \sum_{m} C^{m}_{2\mathrm{pt}}(t) \left[\frac{Z'^{\dagger\mathrm{snk}}_m(k^2)}{Z^{\dagger\mathrm{snk}}_m(k^2)} + \frac{Z'^{\mathrm{src}}_m(k^2)}{Z^{\mathrm{src}}_m(k^2)} - \frac{1}{2E_m^2(k^2)} - \frac{t}{2E_m(k^2)} \right], \tag{10}$$

where Z' is the k^2 derivative of the overlap factors. In particular, $Z' = 0$ for point sources and sinks since a Dirac delta function provides equal support for all momenta.

3. 4-momentum derivatives

The lattice correlation functions and the corresponding spectral decomposition is computed by directly taking the 3-momentum derivative. In general however, the radius of a hadron, or more generally the form factor, depends on the 4-momentum transfer squared $Q^2 = -q^2$ where

$$-q \equiv \begin{pmatrix} E_n(k^2) - M_m \\ 0 \\ 0 \\ k \end{pmatrix}, \tag{11}$$

which we again, assume that the final state hadron is at rest, such that $M_m = E_m(0)$. As a result, the Q^2 derivative of the matrix element is related to the k^2 derivative through the chain rule,

$$\frac{\partial}{\partial k^2}\Gamma_{mn} = \frac{\partial Q^2}{\partial k^2}\frac{\partial}{\partial Q^2}\Gamma_{mn} = \frac{M_m}{\sqrt{M_n^2 + k^2}}\frac{\partial}{\partial Q^2}\Gamma_{mn}, \tag{12}$$

where M_n and M_m is respectively the rest mass of the initial and final state hadron.

C. Reparameterization

Dependence on the inverse of the matrix elements and overlap factors may lead to numerical instability especially when a large number of excited states are included in the fit ansatz. This is due to the fact that *a priori* the sign of the excited state parameters are unknown, and values close to zero may be sampled. In order to improve numerical stability, the following reparameterizations are suggested.

For the two- and three-point correlation function the factors of of E are absorbed into the definition of Z and Γ,

$$C_{2\mathrm{pt}}(t) = \sum_m z_m^{\dagger\mathrm{snk}}(k^2) z_m^{\mathrm{src}}(k^2) e^{-E_m(k^2)t}, \tag{13}$$

$$C_{3\mathrm{pt}}(t,t') = \sum_{m,n} z^{\dagger\mathrm{snk}}(0) g_{mn}(k^2) z_n^{\mathrm{src}}(k^2) \times e^{-E_m(0)(t-t')} e^{-E_n(k^2)t'}, \tag{14}$$

such that

$$z_n \equiv \frac{Z_n(k^2)}{\sqrt{2E_n(k^2)}}, \tag{15}$$

$$g_{mn} \equiv \frac{\Gamma_{mn}(k^2)}{2\sqrt{E_m(0)E_n(k^2)}}. \tag{16}$$

Parameters from the derivative correlation function may be inferred using,

$$C'_{2\mathrm{pt}}(t) = \sum_m C^m_{2\mathrm{pt}}(t)\left[z_m'^{\dagger\mathrm{snk}}(k^2) + z_m'^{\mathrm{src}}(k^2) - \frac{1}{2E_m^2(k^2)} - \frac{t}{2E_m(k^2)}\right], \tag{17}$$

$$C'_{3\mathrm{pt}}(t,t') = C^{mn}_{3\mathrm{pt}}(t,t')\left[g'_{mn}(k^2) + z_n'^{\mathrm{src}}(k^2) - \frac{1}{2E_m^2(k^2)} - \frac{t'}{2E_m(k^2)}\right], \tag{18}$$

where

$$z_n'^{\mathrm{src(snk)}} \equiv \frac{Z_n'^{\mathrm{src(snk)}}(k^2)}{z_n^{\mathrm{src(snk)}}(k^2)\sqrt{2E_n(k^2)}}, \tag{19}$$

$$g'_{mn} \equiv \frac{\Gamma'_{mn}}{2g_{mn}\sqrt{E_m(0)E_n(k^2)}}. \tag{20}$$

This is perhaps the minimal required for this section.

III. CHARGE RADIUS OF THE PROTON

Discuss ensemble information. Show fit on 3296 and 4896 data.

A. Isotropic-clover ensembles

To demonstrate the efficacy of this approach, we perform a preliminary calculation of the connected up-quark contribution of the proton charge radius on two W&M/JLab (William and Mary, and Jefferson Lab) isotropic-clover ensembles []. Both ensembles have a lattice spacing of $\sim$0.12 fm with $\sim$400 MeV pion masses. In both cases, 200 configurations averaged over two sources are used to resolve the statistical uncertainty. The two ensembles differ in their spatial volumes, with length $N_l = \{32, 48\}$ l.u. (lattice units) corresponding to $m_\pi L \sim \{7.7, 11.5\}$, and are distinguished in the rest of the paper by the labels 'l3296' and 'l4896' respectively.

The three-point correlation functions are constructed using a 'sequential propagator' with sink-locations at $T = \{10, 14\}$.

B. Correlator analysis

IV. CONCLUSIONS AND OUTLOOK

This is a great paper. Please publish. Thanks.

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