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<th>Citation</th>
<th>Savage, Martin J. et al. &quot;Proton-Proton Fusion and Tritium Decay from Lattice Quantum Chromodynamics.&quot; Physical Review Letters 119, 6: 062002 © 2017 American Physical Society</th>
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</thead>
<tbody>
<tr>
<td>As Published</td>
<td><a href="http://dx.doi.org/10.1103/PhysRevLett.119.062002">http://dx.doi.org/10.1103/PhysRevLett.119.062002</a></td>
</tr>
<tr>
<td>Publisher</td>
<td>American Physical Society</td>
</tr>
<tr>
<td>Version</td>
<td>Final published version</td>
</tr>
<tr>
<td>Accessed</td>
<td>Sat Sep 16 00:17:29 EDT 2017</td>
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<tr>
<td>Citable Link</td>
<td><a href="http://hdl.handle.net/1721.1/110935">http://hdl.handle.net/1721.1/110935</a></td>
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Proton-Proton Fusion and Tritium $\beta$ Decay from Lattice Quantum Chromodynamics

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(Received 21 November 2016; revised manuscript received 26 January 2017; published 10 August 2017)

The nuclear matrix element determining the $pp \rightarrow de^+\nu_e$ fusion cross section and the Gamow-Teller matrix element contributing to tritium $\beta$ decay are calculated with lattice quantum chromodynamics for the first time. Using a new implementation of the background field method, these quantities are calculated at the SU(3) flavor–symmetric value of the quark masses, corresponding to a pion mass of $m_\pi \sim 806$ MeV. The Gamow-Teller matrix element in tritium is found to be $0.979(03)(10)$ at these quark masses, which is within 2σ of the experimental value. Assuming that the short-distance correlated two-nucleon contributions to the matrix element (meson-exchange currents) depend only mildly on the quark masses, as seen for the analogous magnetic interactions, the calculated $pp \rightarrow de^+\nu_e$ transition matrix element leads to a fusion cross section at the physical quark masses that is consistent with its currently accepted value. Moreover, the leading two-nucleon axial counterterm of pionless effective field theory is determined to be $\Lambda_{1A} = 3.9(0.2)/(1.0)/(0.4)/(0.9) \text{ fm}^3$ at a renormalization scale set by the physical pion mass, also agreeing within the accepted phenomenological range. This work concretely demonstrates that weak transition amplitudes in few-nucleon systems can be studied directly from the fundamental quark and gluon degrees of freedom and opens the way for subsequent investigations of many important quantities in nuclear physics.

DOI: 10.1103/PhysRevLett.119.062002

Weak nuclear processes play a central role in many settings, from the instability of the neutron to the dynamics of core-collapse supernovae. In this work, the results of the first lattice quantum chromodynamics (LQCD) calculations of two such processes are presented, namely, the $pp \rightarrow de^+\nu_e$ fusion process and tritium $\beta$ decay. The $pp \rightarrow de^+\nu_e$ process is centrally important in astrophysics as it is primarily responsible for initiating the proton-proton fusion chain reaction that provides the dominant energy production mechanism in stars like the Sun. Significant theoretical effort has been expended in refining calculations of the $pp \rightarrow de^+\nu_e$ cross section at the energies relevant to solar burning, and progress continues to be made with a range of techniques [1–10], as summarized in Ref. [11]. This process is related to the $\tau d \rightarrow nne^+$ neutrino-induced deuteron-breakup reaction [12–14], relevant to the measurement of neutrino oscillations at the Sudbury Neutrino Observatory [15,16], and to the muon capture reaction $\mu^-d \rightarrow nne_\mu$, which is the focus of current investigation in the MuSun experiment [17]. The second process studied in this work, tritium $\beta$ decay, is a powerful tool for investigating the weak interactions of the Standard Model and plays an important role in the search for new physics. The superallowed process $^3\text{H} \rightarrow ^3\text{He} e^-\bar{\nu}$ is theoretically clean and is the simplest semileptonic weak decay of a nuclear system. In contrast to $pp$ fusion, this decay has been very precisely studied in the laboratory (see Ref. [18] for a review) and provides important constraints on the antineutrino mass [19]. Tritium $\beta$ decay is also potentially sensitive to sterile neutrinos [20,21] and to interactions not present in the Standard Model [21–24]. Although the dominant contributions to the decay rate are under theoretical control as this is a superallowed process, the Gamow-Teller (GT) contribution (axial current) is somewhat more challenging to address than the Fermi ($F$) contribution (vector current). Improved constraints on multibody contributions to the GT matrix element will translate into reduced uncertainties in predictions for decay rates of larger nuclei and are a first step towards understanding the quenching of $g_A$ in nuclei [25–27], a long-standing problem in nuclear theory.
In this Letter, LQCD is used to study the $pp \rightarrow de^+\nu_e$ fusion process and the Gamow-Teller matrix element contributing to tritium $\beta$ decay for the first time, albeit at unphysically large values of the light quark masses and neglecting the effects of isospin breaking and electromagnetism. This is accomplished using a new algorithm for implementing background fields, which is superior to existing methods. Further, the quantities of interest are extracted at high precision using a refined analysis strategy made possible by this new approach. For $pp \rightarrow de^+\nu_e$, the deviations from the single-nucleon contributions are small but are well resolved with the new technique. The leading two-nucleon axial counterterm of pionless effective field theory ($\sigma$EFT), $L_{1,A}$, is determined. The axial coupling of $^3\text{H}$ that determines the matrix element for $^3\text{H} \rightarrow ^3\text{He}e^{-}\overline{\nu}$ in the isospin limit is found to be slightly smaller than that of the proton and is consistent with previous phenomenological estimates [6].

Background axial fields.—Background field techniques were first used in LQCD in the pioneering works of Ref. [28] and Refs. [29,30] in the cases of axial and magnetic fields, respectively. Significant effort has been applied to using background electromagnetic fields to extract magnetic moments and electromagnetic polarizabilities of hadrons [31–35] and nuclei [36–38], as well as the magnetic transition amplitude for the $np \rightarrow dy$ process [39]. Very recently, axial background fields have been employed to extract the axial charge of the proton [40,41], and generalizations to nonzero momentum transfer [42–44] have been used [45] to access the axial form factor of the nucleon.

In this work, a new method is used to generate hadronic correlation functions order by order in the background field. In the standard approach, correlation functions are constructed from the contraction of quark propagators that are modified by the presence of a background field. The same effect can be achieved by directly constructing correlation functions order by order in the background field strength parameter $\lambda$. The axial current renormalization factor $Z_A$ was determined from computations of the vector current in the proton, noting that $Z_A = Z_V + \mathcal{O}(a)$ and assigning a $5\%$ systematic uncertainty associated with lattice-spacing artifacts (statistical uncertainties are negligible). A determination that removes the leading lattice-spacing artifacts leads to $Z_A = 0.8623(01)$ [51,52] at a pion mass of $m_\pi \sim 317$ MeV.

The proton axial charge.—The simplest matrix element of the isovector axial current determines the axial charge of the proton. The correlation function $C^{(p)}_{\lambda,u,\gamma_d}(t)$ is at most quadratic in $\lambda_u$ and linear in $\lambda_d$ when constructed from the compound propagators $S^{(u)}_{\lambda_u/3\gamma_d}(x,y)$ and $S^{(d)}_{\lambda_d/3\gamma_d}(x,y)$, as the proton has two valence $u$ quarks and one valence $d$ quark. Consequently, using at least one (two) nonzero value(s) of $\lambda_{d(u)}$ enables extraction of the axial current matrix element as the linear response by using suitable polynomial fits. The difference of the up-quark and down-quark matrix elements can be used to construct the desired three-point function containing the isovector axial current. This can then be combined with the zero-field two-point

\[
C^{(h)}_{\lambda_u,\gamma_d}(t) = \sum_x \langle 0|\chi^+_h(x,t)\chi^+_h(0)|0\rangle_{\lambda_u,\gamma_d},
\]

where $\langle \cdots \rangle_{\lambda_u,\gamma_d}$ denotes the expectation value determined using the compound propagators. The interpolating operators for hadrons and nuclei, $\chi$, are those previously used to study the spectroscopy of these systems [47,48]. By construction, $C^{(h)}_{\lambda_u,\gamma_d}(t)$ is a polynomial of maximum order $h_u^N_d h_d^{N_d}$ in the field strengths, where $N_u(d)$ is the number of up (down) quarks in the particular interpolating operator.

Details of the LQCD calculation.—The calculations presented below used an ensemble of gauge-field configurations generated with a clover-improved fermion action [49] and a Lüscher-Weisz gauge action [50]. The ensemble was generated with $N_f = 3$ degenerate light-quark flavors with masses tuned to the physical strange quark mass, producing a pion mass of $m_\pi \sim 806$ MeV, with a volume of $L^3 \times T = 32^3 \times 48$ and a lattice spacing of $a \sim 0.145$ fm (as determined from $\Upsilon$ spectroscopy). For these calculations, 437 configurations, with a spacing of ten trajectories between configurations, were used. Correlation functions were computed for $h = \{p,n,d,nn,np(1)S_0\}$, $pp$, $^3\text{H}$, $^3\text{He}$ from propagators generated from a smeared source and either a smeared (SS) or point (SP) sink. Sixteen different source locations were averaged over on each configuration. Compound propagator and correlation functions were calculated at six different values of the background field strength parameter $\lambda = \{\pm 0.05, \pm 0.1, \pm 0.2\}$. The axial current renormalization factor $Z_A = 0.867(43)$ was determined from computations of the vector current in the proton, noting that $Z_A = Z_V + \mathcal{O}(a)$ and assigning a $5\%$ systematic uncertainty associated with lattice-spacing artifacts (statistical uncertainties are negligible). A determination that removes the leading lattice-spacing artifacts leads to $Z_A = 0.8623(01)$ [51,52] at a pion mass of $m_\pi \sim 317$ MeV.
function to form a ratio that asymptotes to the desired axial charge at late times, namely,

\[ R_p(t) = \frac{C_{\lambda a,\lambda d}(p)_{O(\lambda a)} - C_{\lambda a,0,\lambda d}(p)_{O(\lambda a)}}{C_{\lambda a,0,\lambda d}(p)_{O(\lambda a)}}, \]

where the ratios are spin-weighted averages, and \( |O(\lambda a)| \) extracts the coefficient of \( \lambda_q \) in the preceding expression. Then,

\[ R_p(t) \equiv R_p(t + 1) - R_p(t) \rightarrow \frac{g_A}{Z_A}, \]

where corrections to this relation from backwards propagating states originating from the finite extent of the time direction are suppressed by at least \( e^{-2m_0^2T/\beta} \sim 10^{-7} \) in the signal region in the present set of calculations. The effective-\( g_A \) plots resulting from the correlator differences are shown in Fig. 1, along with the result of a combined constant fit to the SS and SP ratios that extracts \( g_A/Z_A \) from the late-time asymptote. The extracted value is \( g_A/Z_A = 1.298(2)(7) \), where the first uncertainty is statistical (determined from a bootstrap analysis) and the second is systematic (arising from choices of fit ranges in both the field strengths and temporal separation as well as from differences in analysis techniques). Including the renormalization factor yields an axial charge of \( g_A = 1.13(2)(7) \), which is consistent with previous determinations from standard three-point function techniques at this pion mass [53,54].

The GT matrix element for tritium \( \beta \) decay.—The half-life of tritium, \( t_{1/2} \), is related to the \( F \) and GT matrix elements by [1]

\[ \frac{1 + \delta_R}{K/G_F^2} t_{1/2} = \frac{1}{(F^2 + f_A/f_V g_A^2 (GT)^2).} \]

where the factors on the left-hand side are known precisely from theory or experiment. On the right-hand side, \( f_A/V \) denote known Fermi functions [55] and \( (F) \) and \( \langle GT \rangle \) are the \( F \) and GT reduced matrix elements, respectively. The Ademollo-Gatto theorem [56] implies \( (F) \sim 1 \), modified only by second-order isospin breaking and by electro-magnetic corrections. However, \( \langle \text{He} | \gamma \gamma \gamma r^+ q | 3^H \rangle = \bar{u} r \gamma_5 \gamma^+ u g_A (GT) \) (assuming vanishing electron mass and at vanishing lepton momentum) is less constrained, and its evaluation is the focus of this section.

By isospin symmetry, the spin-averaged GT matrix element for \( 3^H \rightarrow 3^He^{-}e^+ \) is related to the axial charge of the triton, \( g_A(3^H) \), when the light quarks are degenerate and in the absence of electromagnetism. Analogous to \( R_p(t) \) in Eq. (3), the ratio \( R_H(t) \) of correlation functions in background fields is constructed such that, analogous to Eq. (4), \( R_H(t) \rightarrow g_A(3^H)/Z_A \) in the large-time limit. The analysis of these correlation functions is more complex than for the proton because the triton has four up quarks and five down quarks and the correlators are thus quartic and quintic polynomials in \( \lambda_u, \lambda_d \), respectively. Polynomial fits to the calculated correlation functions are sufficient to extract the terms linear in \( \lambda_u, \lambda_d \), respectively. Results for \( R_H(t) \) are shown in Fig. 2 along with a constant fit to the asymptotic value \( g_A(3^H)/Z_A \). Also shown in Fig. 2 is \( \langle GT \rangle (t) = R_H(t)/R_p(t) \), which is independent of \( Z_A \), and the fit to its asymptotic value \( g_A(3^H)/g_A \). Analyses of these ratios lead to

\[ \frac{g_A(3^H)}{Z_A} = 1.272(6)(22), \quad \frac{g_A(3^H)}{g_A} = 0.979(3)(10), \]

where the first uncertainties are statistical and the second arise from systematics as described for \( g_A \). The result for \( g_A(3^H)/g_A \) is quite close to the precise, experimentally determined value of \( g_A(3^H)/g_A = 0.9511(13) [6] \) at the physical quark masses. In the context of \( xEFT \), the short-distance two-nucleon axial-vector operator, with coefficient \( L_{1,A} [4] \), is expected to give the leading contribution to the difference of this ratio from unity [57].

The low-energy proton-proton fusion cross section.—The low-energy cross section for \( pp \rightarrow de^+\bar{\nu} \) is dictated by the matrix element

\[ \langle d|\bar{\nu}|p p \rangle = g_A C_7 \sqrt{\frac{32\pi}{3}} \Lambda(p) \delta_{jk}, \]

where \( A^g_\pm(x) \) is the axial current with isospin and spin components \( a \) and \( k \), respectively, \( j \) is the deuteron spin index, \( C_7 \) is the Sommerfeld factor, and \( \gamma \) is the deuteron binding momentum. The quantity \( \Lambda(p) \) has been calculated.
mixing between the two-nucleon channels induced by an isovector magnetic field was treated by diagonalizing a (channel-space) matrix of correlators and determining the splittings between energy eigenvalues. This provided access to the matrix element dictating the transition matrix element in the finite lattice volume:

\[
C_{\lambda_u,\lambda_d=0}^{J_z=3}(t) = \lambda_u \sum_{\tau=0}^{t} \sum_{x,y} \langle 0 | \chi_{Jz}^{3} (x, t) A^{\gamma}_{S} (y, \tau) \chi_{Jz}^{1} S_{0} (0) | 0 \rangle
+ c_2 \lambda_u^2 + c_3 \lambda_u^3, \tag{10}
\]

where \( \chi_{Jz}^{3} (x, t) \) is an interpolating field for the \( J_z = 3 \) \( (I_z = 0) \) component of the \( J_z = 3 \) \( 1 \) channel, \( A^{\gamma}_{S} = \bar{u} \gamma_{\gamma} \gamma_{5} u \), and \( c_{2,3} \) are irrelevant terms. Calculations of the background field correlators at three or more values of \( \lambda_u \) allow for the extraction of the term that is linear in \( \lambda_u \). A similar procedure yields the term that is linear in \( \lambda_d \) from background fields coupling to the \( d \) quark. Taking the difference of the ratios of these terms to the corresponding zero-field two-point functions determines the transition matrix element in the finite lattice volume:

\[
R_{S_1, S_0}^{I_z=0, I_z=3}(t) = \frac{C_{\lambda_u,\lambda_d=0}^{J_z=3}(t) |_{\langle 0 |(\lambda_u) \rangle} - C_{\lambda_u,\lambda_d=0}^{J_z=3}(t) |_{\langle 0 |(\lambda_d) \rangle}}{\sqrt{C_{\lambda_u=0,\lambda_d=0}^{J_z=3}(t) C_{\lambda_u=0,\lambda_d=0}^{J_z=3}(t)}}, \tag{11}
\]

Consequently, the difference between ratios at neighboring timeslices determines the isovector matrix element:

\[
R_{S_1, S_0}^{I_z=0, I_z=3}(t) \equiv R_{S_1, S_0}^{I_z=0, I_z=3}(t + 1) - R_{S_1, S_0}^{I_z=0, I_z=3}(t) \rightarrow_{t \rightarrow \infty} \frac{3S_1; I_z = 0 | A^{3}_{S} | S_{0}; I_z = 0 \rangle}{Z_A}, \tag{12}
\]

in the limit where \( \Delta E = E_d - E_p \) is small (as is the case with the quark masses used in this calculation [47]), and when the contributions from excited states are suppressed. This quantity, measured with both SS and SP correlators, is shown in Fig. 3, along with the extracted value of the axial matrix element \( \langle 3S_1; J_z = 0 | A^{3}_{S} | S_{0}; I_z = 0 \rangle / Z_A = 2.568(5)(31) \), where the first uncertainty is statistical and the second is a systematic encompassing choices of fit ranges in time, field strength, and variations in analysis techniques. The latter includes an estimate of the violation of Wigner’s SU(4) symmetry, contributing an uncertainty of \( O(1/N_c^3) \sim 1\% \) to the extraction of the matrix element based on the large \( N_c \)-limit. At the pion mass of this study, the initial and final two-nucleon states are deeply bound.
degeneracy of the in the lower panel of Fig. 3. Taking advantage of the near-volume matrix elements and transition amplitudes requires or only weakly bound, the connection between finite-volume two-nucleon quantity to show that this correlated difference leads directly to the additional 1\% uncertainty from Wigner symmetry breaking is only the statistical and fitting systematic uncertainties (the correspond to fits to the asymptotic plateau behavior and include only the statistical and fitting systematic uncertainties (the additional 1\% uncertainty from Wigner symmetry breaking is not represented in the bands).

and the finite-volume effects in the matrix elements are negligible [62,63]. At lighter values of the quark masses, where the np\{(S_0)\} system and/or the deuteron is unbound or only weakly bound, the connection between finite-volume matrix elements and transition amplitudes requires the framework developed in Refs. [62,63].

To isolate the two-body contribution, the combination \( L^{sd}_{1A} / Z_A \), where the three uncertainties are

\[
\frac{L^{sd}_{1A}}{Z_A} = \langle \sum_{i=1}^{3} S_i; J_z = 0| A_{3}^{i} S_0; J_z = 0 \rangle - 2g_A
\]

\[= -0.011(01)(15). \tag{13} \]

where the first uncertainty is statistical and the second encompasses fitting and analysis systematics.

In light of the mild quark-mass dependence of the analogous short-distance, two-body quantity contributing to np \( \rightarrow dy \) [39], \( L^{sd}_{1A} \) is likely to be largely insensitive to the pion mass between \( m_\pi \sim 806 \text{ MeV} \) and its physical value. This approximate independence and the associated systematic uncertainty will need to be refined in subsequent calculations. Based on this expectation, the result obtained here at \( m_\pi \sim 806 \text{ MeV} \) is used to estimate the value of \( L^{sd}_{1A} \) at the physical pion mass by including an additional 50\% additive uncertainty. Propagating this uncertainty through Eq. (8), the threshold value of \( \Lambda(p) \) in this system at the physical quark masses is determined to be 

\[\Lambda(0) = 2.659(2)(9)(5), \]

where the three uncertainties are the statistical uncertainty, the fitting and analysis systematic uncertainty, and the quark-mass extrapolation systematic uncertainty, respectively. Uncertainties in the scattering parameters and other physical mass inputs are also propagated and included in the systematic uncertainty. This result is remarkably close to the currently accepted, precise phenomenological value \( \Lambda(0) = 2.65(1) \) [11] (see also Ref. [57]). The N^2LO relation of Ref. [4], when enhanced by the summation of the effective ranges to all orders using the dibaryon field approach [10,59,60], gives

\[\Lambda(0) = 2.62(1) + 0.0105(1)L^{sd}_{1A}, \]

enabling a determination of the \( \pi \)EFT coupling.

\[L^{sd}_{1A} = 3.9(0.2)(1.0)(0.4)(0.9) \text{ fm}^3, \tag{14} \]

at a renormalization scale \( \mu = m_\pi \). The four uncertainties are the statistical uncertainty, the fitting and analysis systematic uncertainty, the mass extrapolation systematic uncertainty, and a power-counting estimate of higher order corrections in \( \pi \)EFT, respectively. This value is also very close to previous phenomenological estimates, as summarized in Refs. [11,14].

Summary.—The primary results of this work are the isovector axial-current matrix elements in two- and three-nucleon systems calculated directly from the underlying theory of the strong interactions using lattice QCD (see also the Supplementary Material [64]). These matrix elements determine the cross section for the pp fusion process pp \( \rightarrow d\pi \nu \) and the Gamow-Teller contribution to tritium \( \beta \) decay, \( ^3\text{H} \rightarrow ^3\text{He} e^- \bar{\nu} \). While the calculations are performed at unphysical quark masses corresponding to \( m_\pi \sim 806 \text{ MeV} \) and at a single lattice spacing and volume, the mild mass dependence of the analogous short-distance quantity in the np \( \rightarrow dy \) magnetic transition enables an estimate of the pp \( \rightarrow d\pi \nu \) matrix element at the physical values of the quark masses, and the results are found to agree within uncertainties with phenomenology. Future LQCD calculations, including electromagnetism beyond Coulomb effects, at lighter quark masses with isospin splittings, larger volumes, and finer lattice spacings, making use of the new techniques that are introduced here, will enable extractions of these axial matrix elements with fully quantified uncertainties and will be important for phenomenology, providing increasingly precise values for the pp fusion cross section and GT matrix element in tritium \( \beta \) decay.

Beyond the current study, background axial-field calculations also allow the extraction of second-order, as well as momentum-dependent, responses to axial fields.
Second-order responses are important for determining nuclear $\beta\beta$-decay matrix elements, both with and without (for a light Majorana neutrino) the emission of associated neutrinos [70]. Momentum-dependent axial background fields will allow the determination of nuclear effects in neutrino-nucleus scattering. In both cases, LQCD calculations of these quantities in light nuclei will provide vital input with which to constrain the nuclear many-body methods that are used to determine the matrix elements for these processes in heavy nuclei.

We would like to thank Jiunn-Wei Chen and Peter Kammel for several interesting discussions. This research was supported in part by the National Science Foundation under Grant No. NSF PHY11-25915, and S. R. B., Z. D., W. D., M. J. S., P. E. S., B. C. T., and M. L. W. acknowledge the Kavli Institute for Theoretical Physics for hospitality during completion of this work. Calculations were performed using computational resources provided by National Energy Research Supercomputing Center (supported by U.S. Department of Energy Grant No. DE-AC02-05CH11231), and by the USQCD Collaboration. This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. The PRACE Research Infrastructure resources at the Très Grand Centre de Calcul and Barcelona Supercomputing Center were also used. Parts of the calculations used the CHROMA software suite [71]. S. R. B was partially supported by National Science Foundation Continuing Grant No. PHY1206498 and by the U.S. Department of Energy through Grant No. DE-SC001347. E. C. was supported in part by the USQCD SciDAC project, the U.S. Department of Energy through Grant No. DE-SC0001347. E. C. was supported in part by the USQCD SciDAC project, the U.S. Department of Energy through Grant No. DE-AC02-05CH11231, and by the USQCD Collaboration. This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. The PRACE Research Infrastructure resources at the Très Grand Centre de Calcul and Barcelona Supercomputing Center were also used. Parts of the calculations used the CHROMA software suite [71]. S. R. B was partially supported by National Science Foundation Continuing Grant No. PHY1206498 and by the U.S. Department of Energy through Grant No. DE-SC001347. E. C. was supported in part by the USQCD SciDAC project, the U.S. Department of Energy through Grant No. DE-AC02-05CH11231, and by the USQCD Collaboration. This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

[64] Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.119.062002 provides additional details pertaining to the correlation functions, axial current renormalization, effective masses, uncertainty propagation in EFT matching, and quark mass dependence and also includes Refs. [65–69].