

Neutrinoless double beta decay from lattice QCD: The short-distance $\pi^- \rightarrow \pi^+ e^- e^-$ amplitude

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This work presents a determination of potential short-distance contributions to the unphysical $\pi^- \rightarrow \pi^+ e^- e^-$ decay through lattice QCD calculations. The hadronic contributions to the transition amplitude are described by the pion matrix elements of five Standard Model effective field theory operators, which are computed on five ensembles of domain-wall fermions with $N_f = 2 + 1$ quark flavors with a range of heavier-than-physical values of the light quark masses. The matrix elements are extrapolated to the continuum, physical light-quark mass, and infinite volume limit using a functional form derived in chiral effective field theory (χ EFT). This extrapolation also yields the relevant low-energy constants of χ EFT, which are a necessary input for χ EFT calculations of neutrinoless double beta decay of nuclei.

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I. INTRODUCTION

Neutrinoless double beta ($0\nu\beta\beta$) decay, if observed, would unambiguously reveal the existence of physics beyond the Standard Model (BSM) [1]. In particular, it would imply that the difference between baryon number and lepton number ($B - L$) is not a fundamental symmetry of the Universe [2], and would prove that the neutrino is a Majorana particle [3]. Moreover, observation of $0\nu\beta\beta$ decay would provide additional information about the matter-antimatter asymmetry in the Universe [4], which may help to explain baryogenesis and further constrain the neutrino masses [5].

As such, experiments are underway worldwide to search for $0\nu\beta\beta$ decay, the most sensitive of which study ^{76}Ge and ^{136}Xe and constrain the half-lives of $0\nu\beta\beta$ decay in each isotope to be greater than 10^{26} years [6–10]. Understanding the implication of these constraints for possible BSM physics scenarios requires input in the form of nuclear matrix elements (NMEs); which NMEs are relevant depends on the underlying mechanism of $0\nu\beta\beta$ decay. These mechanisms can be broadly divided into two categories: long-distance mechanisms, in which the decay is induced by a nonlocal interaction mediated by a light particle of mass much less than the hadronic scale [11,12]; and short-distance mechanisms, in which the decay is mediated by a heavy particle that can be integrated out

in effective field theory (EFT) to generate contact interactions [13,14]. In extensions of the Standard Model, long-distance mechanisms are typically assumed to be generated by the dimension-5 Weinberg operator, in which the mediating particle is generally a light Majorana neutrino (although other scenarios have been considered) [15–18], while short-distance mechanisms are described by operators of dimension greater than or equal to 9 [19]. The dominant mechanism of $0\nu\beta\beta$ decay will determine the scale Λ_{LNV} at which lepton-number violating physics is observed. In particular, if $0\nu\beta\beta$ decay is primarily described by a long-distance mechanism, then $\Lambda_{\text{LNV}} \gg 1$ TeV [20], while if $0\nu\beta\beta$ decay is primarily described by a short-distance mechanism, $\Lambda_{\text{LNV}} \sim 1$ TeV [21,22]. Both cases must be understood in order to draw conclusions about the underlying BSM physics from any experimental detection of $0\nu\beta\beta$ decay.

Calculations of long- and short-distance $0\nu\beta\beta$ decay matrix elements have been performed with nuclear many-body methods [21,23]. These techniques are currently the only theoretical methods which can provide insight into $0\nu\beta\beta$ decay in nuclear isotopes which are experimentally relevant. The requisite NMEs for the long- and short-distance $0\nu\beta\beta$ decay of ^{48}Ca , ^{76}Ge , and ^{136}Xe have been computed, although large model dependence in the calculated NMEs remains a challenge for these techniques [6,7,24–26]. To improve these calculations, connection to the Standard Model is required.

Lattice quantum chromodynamics (LQCD) is the only known method with which to compute NMEs directly from the underlying quark and gluon degrees of freedom. However, current LQCD calculations of nuclei suffer from a signal-to-noise problem [27,28] and a factorial increase in

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the number of quark contractions with atomic number [29], which make calculations of phenomenologically relevant nuclei impractical in the absence of new algorithms and approaches. Instead of direct computation of large nuclei, recent work uses EFT [16,22,30–33] to relate LQCD calculations of simpler processes such as the unphysical mesonic transition $\pi^- \rightarrow \pi^+ e^- e^-$ and the two-nucleon $0\nu\beta\beta$ decay $n^0 n^0 \rightarrow p^+ p^+ e^- e^-$ to nuclear $0\nu\beta\beta$ decay. Studies of the $\pi^- \rightarrow \pi^+ e^- e^-$ transition in particular do not incur the technical challenges faced by LQCD calculations of nuclei. The long-distance pion matrix elements have been computed directly using LQCD with a domain-wall fermion action [34,35]. The associated short-distance pion matrix elements have been calculated from LQCD input with two approaches: relating the desired matrix elements to kaon-mixing matrix elements, assuming $SU(3)$ chiral symmetry [36], and computing the pion matrix elements directly using LQCD with a mixed action [37].

This work presents a direct LQCD computation of the $\pi^- \rightarrow \pi^+ e^- e^-$ matrix elements of the leading short-distance (dimension-9) operators, performed for $m_e = 0$ and at threshold. This calculation uses domain-wall fermions, as their chiral symmetry properties yield matrix elements that have a simple renormalization structure. There is a mild tension between the results of the present calculation and the previous mixed-action LQCD calculation of the same matrix elements in Ref. [37], which may be due to the differences in the action used in each calculation. The ensembles used in this calculation are the same as those used in the first lattice computation of the long-distance $\pi^- \rightarrow \pi^+ e^- e^-$ amplitude mediated by light Majorana neutrino exchange [34]. As such, both the long and short-distance contributions to $\pi^- \rightarrow \pi^+ e^- e^-$ have now been computed in a consistent framework, allowing conclusions to be drawn regarding the relative importance of the two potential contributions, as discussed in Sec. IV.

The remainder of this paper is organized as follows. Section II details the EFT framework for the short-distance $\pi^- \rightarrow \pi^+ e^- e^-$ decay and the LQCD calculation of the hadronic part of the transition amplitude. Section III describes the procedure used to extrapolate the renormalized LQCD matrix elements to the physical point using a model based on chiral EFT (χ EFT), and presents results for the extrapolated matrix elements and the extracted χ EFT low-energy constants (LECs). Section IV summarizes the results and presents an outlook.

II. SHORT-DISTANCE MATRIX ELEMENTS

A. Short-distance operators

In the Standard Model EFT (SMEFT) framework, the Standard Model enters as the renormalizable sector of a nonrenormalizable theory [38]. Potential short-distance contributions to $\pi^- \rightarrow \pi^+ e^- e^-$ are induced by physics at the scale $\Lambda_{\text{LNV}} \gtrsim v$, where $v = 247$ GeV is the electroweak

scale set by the Higgs vacuum expectation value and described in the SMEFT by operators with mass dimension greater than 4. At the quark level, any SMEFT operator that contributes to $0\nu\beta\beta$ decay must induce the process $dd \rightarrow uue^- e^-$. Every such operator must therefore contain at least six fermion fields, and so have mass dimension $d \geq 9$, with contributions to the $\pi^- \rightarrow \pi^+ e^- e^-$ decay power-suppressed by a factor of $\Lambda_{\text{LNV}}^{d-4}$. The dimension-9 lepton number violating operators thus contribute to the decay at leading order (LO) in inverse powers of Λ_{LNV} .

There are 14 $SU(3)_c \times U(1)_{\text{EM}}$ -invariant dimension-9 SMEFT operators which violate lepton number and may contribute to $\pi^- \rightarrow \pi^+ e^- e^-$; they can be factorized into a 4-quark operator multiplying a leptonic operator. Of these operators, four have corresponding 4-quark operators that transform as Lorentz 4-vectors, and therefore match to the χ EFT operator $\pi(\partial^\mu \pi) \bar{e} \gamma_\mu \gamma_5 e^c + \text{H.c.}$, where the superscript c denotes charge conjugation and π and e represent the pion and electron fields. Integration by parts shows that pionic matrix elements of this operator are proportional to one power of the electron mass and give subleading contributions to the decay $\pi^- \rightarrow \pi^+ e^- e^-$. Of the remaining ten operators, five have corresponding 4-quark operators with positive parity and contribute to $\pi^- \rightarrow \pi^+ e^- e^-$, while the five operators containing 4-quark operators of negative parity do not contribute. Consequently, at LO the decay is described with the Lagrangian

$$\mathcal{L}_{\text{SMEFT}}^{0\nu\beta\beta} = \bar{e} e^c \frac{G_F^2}{\Lambda_{\text{LNV}}} \sum_k c_k \mathcal{O}_k, \quad (1)$$

where G_F is the Fermi coupling constant, c_k are dimensionless Wilson coefficients, and the operator basis $\{\mathcal{O}_k(x)\}$ is

$$\begin{aligned} \mathcal{O}_1(x) &= (\bar{q}_L(x) \tau^+ \gamma^\mu q_L(x)) [\bar{q}_R(x) \tau^+ \gamma_\mu q_R(x)], \\ \mathcal{O}_2(x) &= (\bar{q}_R(x) \tau^+ q_L(x)) [\bar{q}_R(x) \tau^+ q_L(x)] \\ &\quad + (\bar{q}_L(x) \tau^+ q_R(x)) [\bar{q}_L(x) \tau^+ q_R(x)], \\ \mathcal{O}_3(x) &= (\bar{q}_L(x) \tau^+ \gamma^\mu q_L(x)) [\bar{q}_L(x) \tau^+ \gamma_\mu q_L(x)] \\ &\quad + (\bar{q}_R(x) \tau^+ \gamma^\mu q_R(x)) [\bar{q}_R(x) \tau^+ \gamma_\mu q_R(x)], \\ \mathcal{O}_{1'}(x) &= (\bar{q}_L(x) \tau^+ \gamma^\mu q_L(x)) [\bar{q}_R(x) \tau^+ \gamma_\mu q_R(x)], \\ \mathcal{O}_{2'}(x) &= (\bar{q}_R(x) \tau^+ q_L(x)) [\bar{q}_R(x) \tau^+ q_L(x)] \\ &\quad + (\bar{q}_L(x) \tau^+ q_R(x)) [\bar{q}_L(x) \tau^+ q_R(x)], \end{aligned} \quad (2)$$

with $k \in \{1, 2, 3, 1', 2'\}$ [31]. Here $q_L(x)$ and $q_R(x)$ are the left- and right-handed components of the quark field isospin doublet, respectively, and

$$\tau^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad (3)$$

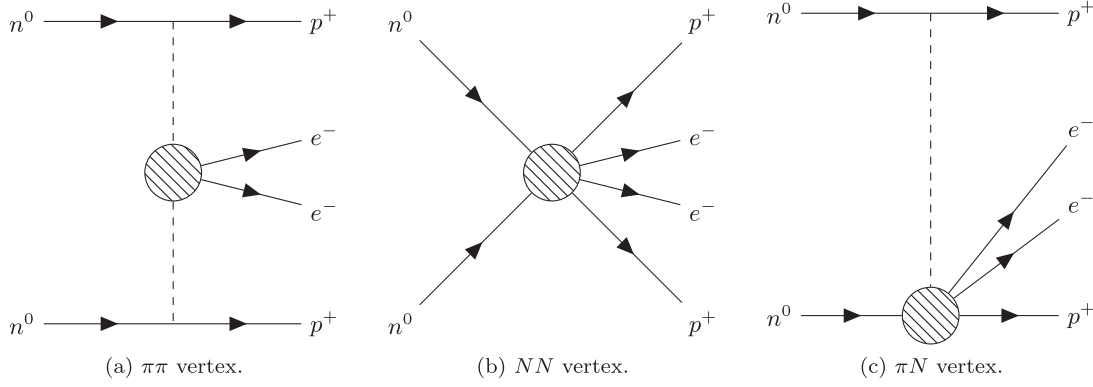


FIG. 1. Diagrams illustrating short-distance contributions to the $n^0 n^0 \rightarrow p^+ p^+ e^- e^-$ $0\nu\beta\beta$ decay in χ EFT. The solid lines denote nucleons or electrons and the dotted lines denote pions. The hatched circles represent EFT operators built from hadronic fields, which are at LO for the $\pi\pi$ vertex diagram, (a) determined by \mathcal{O}_k^χ in Eq. (4). $\pi\pi$ (a) and NN (b) diagrams are the LO χ EFT contributions to $n^0 n^0 \rightarrow p^+ p^+ e^- e^-$.

is the isospin raising operator. The round and square brackets in Eq. (2) denote color contraction: for arbitrary Dirac matrices Γ_1 and Γ_2 , the operators $\{\mathcal{O}_1(x), \mathcal{O}_2(x), \mathcal{O}_3(x)\}$ factor into products of color singlets, $(\bar{u}\Gamma_1 d)[\bar{u}\Gamma_2 d] \equiv (\bar{u}^a \Gamma_1 d^a)(\bar{u}^b \Gamma_2 d^b)$, whereas the operators $\{\mathcal{O}_{1'}(x), \mathcal{O}_{2'}(x)\}$ mix color between the two Dirac bilinear terms, $(\bar{u}\Gamma_1 d)[\bar{u}\Gamma_2 d] \equiv (\bar{u}^a \Gamma_1 d^b)(\bar{u}^b \Gamma_2 d^a)$, where a, b are color indices. The operator basis $\{\mathcal{O}_k(x)\}$ of Eq. (2) is named the BSM basis and is typically used in phenomenological calculations of $0\nu\beta\beta$ decay [33].

Although the $\pi^- \rightarrow \pi^+ e^- e^-$ transition is unphysical, it has phenomenological importance as it can be related to the nuclear decays with χ EFT [22]. In particular, the two-nucleon decay $n^0 n^0 \rightarrow p^+ p^+ e^- e^-$ is induced in χ EFT by the diagrams in Fig. 1 and has LO contributions from the $\pi\pi$ and NN vertices [16,33].¹ The associated effective Lagrangian relevant for $\pi^- \rightarrow \pi^+ e^- e^-$ (i.e., omitting NN and πN operators which do not contribute) is [37]

$$\mathcal{L}_{\chi\text{EFT}}^{0\nu\beta\beta} = \bar{e} e^c \frac{G_F^2}{\Lambda_{\text{LNV}}} \frac{\Lambda_\chi^4}{(4\pi)^2} \frac{f_\pi^2}{8} \left(c_1 \beta_1 \mathcal{O}_1^\chi - \frac{c_2 \beta_2}{2} \mathcal{O}_2^\chi - c_3 \beta_3 \mathcal{O}_3^\chi + c_{1'} \beta_{1'} \mathcal{O}_{1'}^\chi - \frac{c_{2'} \beta_{2'}}{2} \mathcal{O}_{2'}^\chi \right). \quad (4)$$

Here, f_π is the pion decay constant in the chiral limit, $\Lambda_\chi^2 \equiv 8\pi^2 f_\pi^2$ is the scale of chiral symmetry breaking, and \mathcal{O}_k^χ denote the leading χ EFT operators corresponding to \mathcal{O}_k [39]. The χ EFT LECs β_k determine the $\pi\pi$ coupling, and are also essential input to study the nucleonic decay. The β_k can be determined by evaluating the pion matrix elements of the \mathcal{O}_k in LQCD and matching them to the corresponding matrix elements of \mathcal{O}_k^χ in Eq. (4).

¹Earlier work [31] found the $\pi\pi$ contributions to be the sole LO contribution, but the Weinberg power counting used therein did not account for regulator dependence completely.

B. Bare matrix elements

The pion matrix elements of each of the SMEFT operators in Eq. (2) are computed in LQCD using gauge-field ensembles with $N_f = 2 + 1$ quark flavors generated by the RBC/UKQCD Collaboration [40,41]. Each ensemble uses the Shamir kernel [42] for the domain-wall fermion action [43] and the Iwasaki action [44] for the gauge field. The parameters of each ensemble are detailed in Table I, and additional details regarding the ensemble generation can be found in Refs. [40,41,45]. The scale is set using the Wilson flow scale w_0 [46]. The pion mass, m_π , the pion decay constant, f_π , and the axial-vector renormalization constant, \mathcal{Z}_A , for each ensemble were determined in Ref. [34]. In the conventions used here, the physical pion decay constant [47] is $f_\pi^{(\text{phys})} = 130.2$ MeV. The vector renormalization constant, \mathcal{Z}_V , for these ensembles was computed in the chiral limit in Refs. [46,48]. Because $\mathcal{Z}_V \approx \mathcal{Z}_A$, the ensembles exhibit approximate chiral symmetry.

On each ensemble, the time-averaged two-point function

$$C_{2\text{pt}}(t) = \frac{1}{T} \sum_{t_-=0}^{T-1} \sum_{\mathbf{x}, \mathbf{y}} \langle 0 | \chi_\pi(\mathbf{x}, t + t_-) \chi_\pi^\dagger(\mathbf{y}, t_-) | 0 \rangle \quad (5)$$

and three-point functions

$$C_k(t_-, t_x, t_+) = \sum_{\mathbf{x}, \mathbf{y}, \mathbf{z}} \langle 0 | \chi_\pi^\dagger(\mathbf{x}, t_+) \mathcal{O}_k(\mathbf{z}, t_x) \chi_\pi^\dagger(\mathbf{y}, t_-) | 0 \rangle, \quad (6)$$

where the pion interpolating operator $\chi_\pi(x) = \bar{u}(x)\gamma_5 d(x)$ has the quantum numbers of the π^- and $t_+ \geq t_x \geq t_-$, are computed for each operator $\mathcal{O}_k(x)$ in the BSM basis [Eq. (2)]. Wall-source propagators are computed at each available time slice on each configuration, where “wall” denotes projection to vanishing three-momentum in the Coulomb gauge. Note that wall sources are not gauge

TABLE I. Parameters of the gauge-field ensembles used in this study. Each ensemble was generated with two degenerate light quark flavors of mass m_ℓ and one heavy quark flavor of mass m_s . The lattice volumes are $L^3 \times T \times L_s$, with the fifth dimension having L_s sites. Derived quantities are computed in Ref. [34] (the pion mass m_π , the pion decay constant f_π , and the axial current renormalization \mathcal{Z}_A) and Refs. [46,48] (the vector current renormalization \mathcal{Z}_V and the inverse lattice spacing a^{-1}).

Ensemble	am_ℓ	am_s	β	$L^3 \times T \times L_s$	a [fm]	m_π [MeV]	f_π [MeV]	\mathcal{Z}_A	\mathcal{Z}_V
24I	0.01	0.04	2.13	$24^3 \times 64 \times 16$	0.1106(3)	432.2(1.4)	163.72(64)	0.71670(22)	0.71273(26)
	0.005					339.6(1.2)	151.55(62)		
32I	0.008	0.03	2.25	$32^3 \times 64 \times 16$	0.0828(3)	410.8(1.5)	162.02(90)	0.74482(15)	0.7440(18)
	0.006					359.7(1.2)	154.28(70)		
	0.004					302.0(1.1)	147.54(81)		

invariant, hence the need for gauge fixing. The two-point functions [Eq. (5)] are constructed using a wall source propagator at t_- and a wall sink at $t + t_-$, and the three-point functions [Eq. (6)] are constructed using wall source propagators at t_- and t_+ and a point (local) sink at t_x . The explicit Wick contractions are given in Appendix A.

The bare pion matrix elements in lattice units

$$\langle \mathcal{O}_k \rangle \equiv a^4 \langle \pi^+ | \mathcal{O}_k(\mathbf{p} = \mathbf{0}) | \pi^- \rangle = a^4 \sum_{\mathbf{x}} \langle \pi^+ | \mathcal{O}_k(\mathbf{x}, 0) | \pi^- \rangle \quad (7)$$

are extracted from the effective matrix elements

$$O_k^{\text{eff}}(t) \equiv 2m_\pi \frac{C_k(0, t, 2t)}{C_{2\text{pt}}(2t) - \frac{1}{2}C_{2\text{pt}}(T/2)e^{m_\pi(2t-T/2)}}. \quad (8)$$

Subtracting $\frac{1}{2}C_{2\text{pt}}(T/2)e^{m_\pi(2t-T/2)}$ in the denominator of Eq. (8) isolates the backwards-propagating state in the two-point function, and in the $0 \ll t \ll T$ limit $O_k^{\text{eff}}(t)$ asymptotes to $\langle \mathcal{O}_k \rangle$. The effective matrix elements are computed on between 33 and 53 gauge-field configurations for each ensemble (details in Appendix B, Table III), resampled using a bootstrap procedure with $n_b = 50$ bootstrap samples. The spectral decomposition of $O_k^{\text{eff}}(t)$ up to and including the first excited state with energy $m_\pi + \Delta$,

$$O_k^{\text{eff}}(t) = \frac{\langle \mathcal{O}_k \rangle + \mathcal{N}_1^{(k)} e^{-\Delta t} + \mathcal{N}_2^{(k)} e^{-(m_\pi + \Delta)(T-2t)}}{1 + \mathcal{N}_3^{(k)} e^{-2\Delta t} + \mathcal{N}_4^{(k)} e^{-(m_\pi + \Delta)T + 2(2m_\pi + \Delta)t}}, \quad (9)$$

parametrizes the ground and excited-state contributions to $O_k^{\text{eff}}(t)$, where the coefficients $\mathcal{N}_i^{(k)}$ are constants determined by the spectral content of the theory. Equation (9) can be Taylor expanded to first order in $\mathcal{N}_3^{(k)}$ and $\mathcal{N}_4^{(k)}$, yielding

$$\begin{aligned} f_k(t; \langle \mathcal{O}_k \rangle, m^{(k)}, \Delta^{(k)}, A_i^{(k)}) \\ \equiv \langle \mathcal{O}_k \rangle + A_1^{(k)} e^{-\Delta^{(k)} t} + A_2^{(k)} e^{-(m^{(k)} + \Delta^{(k)})(T-2t)} - A_3^{(k)} e^{-2\Delta^{(k)} t} \\ - A_4^{(k)} e^{-(m^{(k)} + \Delta^{(k)})T + 2(2m^{(k)} + \Delta^{(k)})t}. \end{aligned} \quad (10)$$

This function is used to model the temporal dependence of $O_k^{\text{eff}}(t)$, treating $\langle \mathcal{O}_k \rangle, m^{(k)}, \Delta^{(k)}$, and $A_i^{(k)}$ as free parameters.

Fits of $O_k^{\text{eff}}(t)$ to the model of Eq. (10) are performed using a correlated least-squares fit. Each fit is performed over a given range $[t_{\min}, t_{\max}]$, with the covariance matrix obtained from the bootstrapped sample covariance matrix via linear shrinkage with parameter λ [49,50]; the hyperparameters are varied, with $t_{\min} \in [6, 11]$, $t_{\max} \in [30, 32]$, and $\lambda \in \{0.1, 0.2, 0.3, 0.4\}$. Bayesian priors are placed on the model parameters, informed by the results of a two-state fit to $C_{2\text{pt}}(t)$. The priors on the spectral coefficients are set to $A_k^{(i)} = 0.0 \pm 0.1$, where $\mu \pm \sigma$ denotes the normal distribution with mean μ and width σ . To enforce positivity, log-normal priors are chosen for the mass $m_\pi^{(k)}$ and excited state gap $\Delta^{(k)}$ such that $m^{(k)} = m_\pi \pm \delta m_\pi$, where m_π (δm_π) is the mean (standard deviation) of the pion mass (Table I) and $\Delta^{(k)} = 2m_\pi \pm m_\pi$. Statistically indistinguishable results are obtained for $\langle \mathcal{O}_k \rangle$ under variation of all hyperparameters within the ranges described above, and when widths of the priors are inflated by a factor of 2; hence fiducial values of the hyperparameters are chosen as $[t_{\min}, t_{\max}] = [6, 32]$ and $\lambda = 0.1$.² Posterior values for $A_3^{(k)}$ and $A_4^{(k)}$ are found to be $\ll 1$, thus the Taylor expansion in Eq. (10) is valid. The fits have χ^2/dof between 0.10 and 0.73. Fit results and the complete set of fits for each operator on each ensemble with the fiducial hyperparameters are shown in Appendix B. Illustrative fits to data from the 32I, $am_\ell = 0.004$ ensemble with the fiducial hyperparameters are shown in Fig. 2.

C. Renormalization

To make contact with phenomenological calculations, lattice-regulated matrix elements must be renormalized in the $\overline{\text{MS}}$ scheme. In this calculation, the renormalization coefficients are computed nonperturbatively in the RI/sMOM- (γ^μ, γ^μ) (abbreviated as RI γ) scheme [51,52] and

²This choice for λ is statistically the most conservative within the range, as $\lambda = 0$ corresponds to no shrinkage.

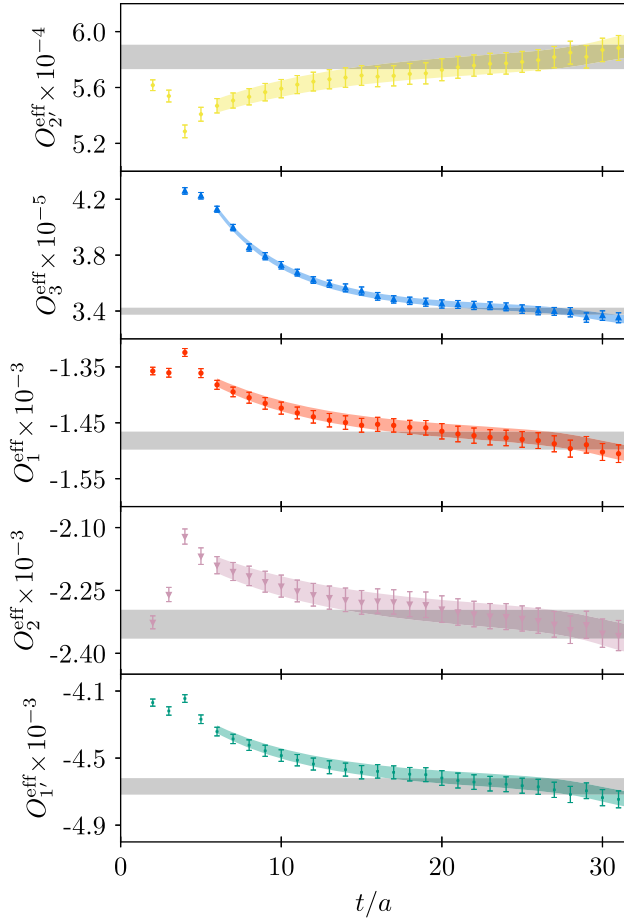


FIG. 2. Effective matrix elements $O_k^{\text{eff}}(t)$ [Eq. (8)] computed on the 32I, $am_\ell = 0.004$ ensemble. Colored bands denote the best-fit band for the corresponding excited-state fit to the model of Eq. (10), with $[t_{\min}, t_{\max}] = [6, 32]$ and $\lambda = 0.1$. The gray band in each panel denotes the extracted value of $\langle O_k \rangle$ [Eq. (10)].

perturbatively matched to $\overline{\text{MS}}$. In terms of the operator basis $\{O_k(x)\}$ [Eq. (2)], the renormalized matrix elements can be expressed as

$$\begin{aligned} O_k^{\overline{\text{MS}}}(x; \mu^2, a) &= Z_{k\ell}^{\overline{\text{MS}}; O}(\mu^2, a) O_\ell(x; a) \\ &= C_{kj}^{\overline{\text{MS}} \leftarrow \text{RI}\gamma; O}(\mu^2, a) Z_{j\ell}^{\text{RI}\gamma; O}(\mu^2, a) O_\ell(x; a), \end{aligned} \quad (11)$$

where sums over repeated indices are implied. Here $O_\ell(x; a)$ denotes the bare operator at lattice spacing a , and

$$C_{kj}^{\overline{\text{MS}} \leftarrow \text{RI}\gamma; O}(\mu^2, a) \equiv Z_{ki}^{\overline{\text{MS}}; O}(\mu^2, a) [Z_{ij}^{\text{RI}\gamma; O}(\mu^2, a)]^{-1} \quad (12)$$

is the multiplicative matching coefficient from the $\text{RI}\gamma$ to $\overline{\text{MS}}$ schemes, computed at one loop in perturbation theory in the strong coupling $\alpha_s(\mu)$ [52,53]. Note that each renormalization coefficient is mass independent and defined in the chiral limit.

The renormalization coefficients, Eq. (11), are conventionally computed in the nonperturbative renormalization (NPR) operator basis, $\{Q_n(x)\}$, which contains different linear combinations of operators than the BSM basis of Eq. (2). Correlation functions involving the color-mixed operators $O_{1'}(x), O_{2'}(x)$ may be rewritten with Fierz identities [54] as combinations of color-unmixed quark bilinears, which simplifies the calculation. The NPR basis is defined in terms of the quark bilinears:

$$\begin{aligned} SS(x) &= (\bar{u}(x)d(x))(\bar{u}(x)d(x)), \\ PP(x) &= (\bar{u}(x)\gamma_5 d(x))(\bar{u}(x)\gamma_5 d(x)), \\ VV(x) &= (\bar{u}(x)\gamma_\mu d(x))(\bar{u}(x)\gamma^\mu d(x)), \\ AA(x) &= (\bar{u}(x)\gamma_\mu \gamma_5 d(x))(\bar{u}(x)\gamma^\mu \gamma_5 d(x)), \\ TT(x) &= \sum_{\mu < \nu} (\bar{u}(x)\gamma_\mu \gamma_\nu d(x))(\bar{u}(x)\gamma^\mu \gamma^\nu d(x)) \end{aligned} \quad (13)$$

as

$$\begin{pmatrix} Q_1(x) \\ Q_2(x) \\ Q_3(x) \\ Q_4(x) \\ Q_5(x) \end{pmatrix} \equiv \begin{pmatrix} VV(x) + AA(x) \\ VV(x) - AA(x) \\ SS(x) - PP(x) \\ SS(x) + PP(x) \\ TT(x) \end{pmatrix}. \quad (14)$$

This basis is related to the positive-parity projection of the BSM basis, Eq. (2), as

$$\begin{pmatrix} Q_1(x) \\ Q_2(x) \\ Q_3(x) \\ Q_4(x) \\ Q_5(x) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 2 & 0 & 0 \\ 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 4 \end{pmatrix} \begin{pmatrix} O_1(x) \\ O_2(x) \\ O_3(x) \\ O_{1'}(x) \\ O_{2'}(x) \end{pmatrix}. \quad (15)$$

The space spanned by $\{Q_n(x)\}$ splits into three irreducible subspaces under chiral symmetry, with bases $\{Q_1(x)\}$, $\{Q_2(x), Q_3(x)\}$, and $\{Q_4(x), Q_5(x)\}$. As both the $\overline{\text{MS}}$ and $\text{RI}\gamma$ schemes obey chiral symmetry, the renormalization coefficients $Z_{nm}^{\overline{\text{MS}}; Q}(\mu^2, a)$ and $Z_{nm}^{\text{RI}\gamma; Q}(\mu^2, a)$, which satisfy analogous equations to Eqs. (11) and (12), each factorize into a direct sum of three block diagonal matrices, each of which spans an irreducible subspace.

To renormalize the NPR basis operators, the four-point functions

$$\begin{aligned} (G_n)^{abcd}(q; a, m_\ell) & \\ & \equiv \frac{1}{V} \sum_x \sum_{x_1, \dots, x_4} e^{i(p_1 \cdot x_1 - p_2 \cdot x_2 + p_1 \cdot x_3 - p_2 \cdot x_4 + 2q \cdot x)} \\ & \quad \times \langle 0 | \bar{d}_d^\delta(x_4) u_c^\gamma(x_3) Q_n(x) \bar{d}_b^\beta(x_2) u_a^\alpha(x_1) | 0 \rangle \end{aligned} \quad (16)$$

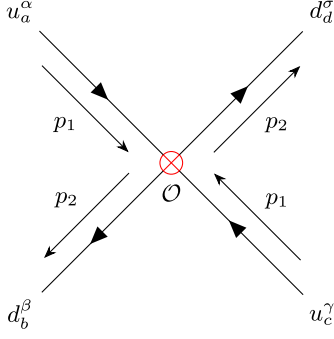


FIG. 3. Kinematics for operator renormalization. The red crossed circle denotes the operator \mathcal{O} which injects momentum $2q$ into the vertex, while the solid lines denote up quarks, with momentum p_1 into the vertex, and down quarks, with momentum p_2 out of the vertex. The momenta are chosen subject to the symmetric constraint, Eq. (17).

are computed on each ensemble, where $V = L^3 \times T$ is the lattice volume and $q = p_2 - p_1$. Latin letters a, b, c, d denote color indices, while Greek letters $\alpha, \beta, \gamma, \delta$ denote Dirac indices. All correlation functions used for the renormalization are computed in the Landau gauge with momentum sources [55] using ten configurations for each ensemble, as the V^2 averaging from the momentum sources significantly reduces noise. The momenta are chosen subject to the symmetric constraint

$$p_1^2 = p_2^2 = q^2 = \mu^2, \quad (17)$$

with the particular choice

$$p_1 = \frac{2\pi}{aL}(-j, 0, j, 0), \quad p_2 = \frac{2\pi}{aL}(0, j, j, 0), \quad (18)$$

with $q = p_2 - p_1$ and $j \in \mathbb{Z}$. The kinematic configuration corresponding to $G_n(q; a, m_\ell)$ is depicted in Fig. 3. Note that with this choice of momentum, each value of q corresponds to a unique value of p_1 and p_2 , hence functions of (p_1, p_2, q) are labeled as functions of q for conciseness. The four-point functions are amputated,

$$\begin{aligned} (\Lambda_n)_{abcd}^{\alpha\beta\gamma\delta}(q) &\equiv (S^{-1})_{aa'}^{\alpha\alpha'}(p_1)(S^{-1})_{cc'}^{\gamma\gamma'}(p_1) \\ &\times (G_n)_{a'b'c'd'}^{\alpha'\beta'\gamma'\delta'}(q)(S^{-1})_{b'b}^{\beta'\beta}(p_2)(S^{-1})_{d'd}^{\delta'\delta}(p_2), \end{aligned} \quad (19)$$

where

$$S(p; a, m_\ell) = \frac{1}{V} \sum_{x,y} e^{ip \cdot (x-y)} \langle 0 | q(x) \bar{q}(y) | 0 \rangle \quad (20)$$

is the Landau-gauge momentum-projected quark propagator. The ensemble dependence of $\Lambda_n(q)$, $G_n(q)$, and $S(p)$ has been suppressed in Eq. (19) for clarity. Projectors

$(P_n)_{abcd}^{\beta\alpha\delta\gamma}$ are introduced to project $(\Lambda_n)_{abcd}^{\alpha\beta\gamma\delta}$ onto the NPR basis for RI γ [52] to yield a matrix of projected four-point functions with components

$$F_{mn}(q; a, m_\ell) \equiv (P_n)_{abcd}^{\beta\alpha\delta\gamma} (\Lambda_m)_{abcd}^{\alpha\beta\gamma\delta}(q; a, m_\ell). \quad (21)$$

The remaining quantities which are computed nonperturbatively on each ensemble are the RI γ quark-field renormalization

$$\left(\frac{\mathcal{Z}_q^{\text{RI}\gamma}}{\mathcal{Z}_V} \right) (\mu^2; a, m_\ell) \Big|_{q^2=\mu^2} = \frac{1}{48} \text{Tr}[\gamma_\mu \Lambda_V^\mu(q)], \quad (22)$$

and the vector and axial-vector-renormalization coefficients, $\mathcal{Z}_V(\mu^2; a, m_\ell)$ and $\mathcal{Z}_A(\mu^2; a, m_\ell)$, whose computation is described in Appendix C. Here $\Lambda_V^\mu(q) = S^{-1}(p_1)G_V^\mu(q)S^{-1}(p_2)$ is the amputated vector three-point function, where

$$\begin{aligned} G_V^\mu(q; a, m_\ell) &= \frac{1}{V} \sum_{x,x_1,x_2} e^{i(p_1 \cdot x_1 - p_2 \cdot x_2 + q \cdot x)} \\ &\times \langle 0 | u(x_1) V^\mu(x) \bar{d}(x_2) | 0 \rangle \end{aligned} \quad (23)$$

is the vector three-point function, with $V^\mu(x) = \bar{u}(x)\gamma^\mu d(x)$ the vector current. The quantities $Z \in \{\mathcal{Z}_q^{\text{RI}\gamma}/\mathcal{Z}_V, F_{nm}\}$ display mild dependence on quark mass and are extrapolated to the chiral limit via a joint fit over ensembles with different masses to the model

$$Z(\mu^2; a, m_\ell) = Z(\mu^2; a) + \tilde{Z}(\mu^2; a)m_\ell \quad (24)$$

where $Z(\mu^2; a)$ and $\tilde{Z}(\mu^2; a)$ are fit coefficients, and $Z(\mu^2; a)$ is understood as the chiral limit of $Z(\mu^2; a, m_\ell)$. Correlations between $\mathcal{Z}_q^{\text{RI}\gamma}/\mathcal{Z}_V$ and F_{nm} on each ensemble are retained in the fits, and the covariance matrix is block diagonal as data from different ensembles is uncorrelated. Fitted values of $Z(\mu^2; a)$ are statistically consistent when a constant model $Z(\mu^2; a, m_\ell) = Z(\mu^2; a)$ is used in place of the linear model of Eq. (24). The full set of extrapolations for $(\mathcal{Z}_q^{\text{RI}\gamma}/\mathcal{Z}_V)(\mu^2; a)$ and $F_{mn}(q; a)$ for both the $a = 0.11$ fm and $a = 0.08$ fm ensembles is shown in Appendix D.

With the definitions above, the NPR-basis renormalization coefficients in the RI γ scheme can be computed as

$$\frac{\mathcal{Z}_{nm}^{\text{RI}\gamma; Q}}{\mathcal{Z}_V^2} (\mu^2; a) \Big|_{\text{sym}} = \left(\frac{\mathcal{Z}_q^{\text{RI}\gamma}(\mu^2; a)}{\mathcal{Z}_V} \right)^2 [F_{nr}^{(\text{tree})} F_{rm}^{-1}(q; a)] \quad (25)$$

where $F_{nr}^{(\text{tree})} \equiv P_r \Lambda_n^{(\text{tree})}$ is the matrix of projections of the tree-level vertex function $\Lambda_n^{(\text{tree})}$, and the notation $|_{\text{sym}}$

denotes evaluation at the symmetric kinematic point, Eq. (17). The renormalization coefficients $Z_{nm}^{\text{RI}^y;Q}(\mu^2; a)/Z_V^2$ are only computed nonperturbatively at scales $\mu_j = \frac{2\pi}{aL} \|(j, j, 0, 0)\|$ corresponding to the lattice momenta given in Eq. (18), where $\|\cdot\|$ denotes the Euclidean norm of the lattice vector. However, the matching coefficients $C_{nm}^{\overline{\text{MS}} \leftarrow \text{RI}^y;Q}(\mu^2, a)$ in Eq. (11) have been computed at $\mu = M \equiv 3$ GeV [52,53], and therefore the renormalization coefficients must be perturbatively evolved from μ_j to M . To minimize the artifacts from truncating the perturbative expansion of the matching coefficients, μ_j must be chosen to lie in the Rome-Southampton window [56,57],

$$\Lambda_{\text{QCD}} \ll \mu_j \ll \left(\frac{\pi}{a}\right), \quad (26)$$

with μ_j taken to satisfy $\mu_j \leq M$ to minimize discretization artifacts. In practice, the scale μ_4 is used for renormalization at both $a = 0.11$ fm and $a = 0.08$ fm, as this is the nearest available scale to M satisfying these constraints.

Numerically, these scales are $\mu_4 = 2.64$ GeV for the $a = 0.11$ fm ensemble and $\mu_4 = 2.65$ GeV for the $a = 0.08$ fm ensemble. Scale evolution from μ_4 to M is performed by integrating the evolution equation,

$$\begin{aligned} \left(\frac{Z_{nm}^{\text{RI}^y;Q}}{Z_V^2}\right)(M; a) &= \left(\frac{Z_{nm}^{\text{RI}^y;Q}}{Z_V^2}\right)(\mu_4; a) \\ &+ \int_{\mu_4}^M \frac{d\mu}{\mu} \gamma_{np}^{\text{RI}^y;Q}(\alpha_s(\mu)) \left(\frac{Z_{pm}^{\text{RI}^y;Q}}{Z_V^2}(\mu; a)\right), \end{aligned} \quad (27)$$

where the NPR basis anomalous dimensions $\gamma_{nm}^{\text{RI}^y;Q}(\alpha_s(\mu))$ have been computed at two-loop order in $\alpha_s(\mu)$ in Ref. [58]. Statistically consistent results for $(Z_{nm}^{\text{RI}^y;Q}/Z_V^2)(M)$ are obtained when μ_3 is instead used as the nonperturbative scale in Eq. (27).

The results for the NPR basis renormalization coefficients, computed at $\mu = 3$ GeV in $\overline{\text{MS}}$, are

$$\begin{aligned} &\left(\frac{Z_{nm}^{\overline{\text{MS}};Q}}{Z_V^2}\right)(\mu^2 = 9 \text{ GeV}^2, a = 0.11 \text{ fm}) \\ &= \begin{pmatrix} 0.90746(43) & 0 & 0 & 0 & 0 \\ 0 & 1.04052(14) & 0.26154(56) & 0 & 0 \\ 0 & 0.05286(12) & 0.95333(75) & 0 & 0 \\ 0 & 0 & 0 & 0.91775(71) & -0.02367(13) \\ 0 & 0 & 0 & -0.28140(66) & 1.13952(35) \end{pmatrix}, \\ &\left(\frac{Z_{nm}^{\overline{\text{MS}};Q}}{Z_V^2}\right)(\mu^2 = 9 \text{ GeV}^2, a = 0.08 \text{ fm}) \\ &= \begin{pmatrix} 0.92625(51) & 0 & 0 & 0 & 0 \\ 0 & 1.03941(31) & 0.27661(50) & 0 & 0 \\ 0 & 0.04203(67) & 0.85916(82) & 0 & 0 \\ 0 & 0 & 0 & 0.84035(87) & -0.01061(40) \\ 0 & 0 & 0 & -0.29928(71) & 1.19362(57) \end{pmatrix}. \end{aligned} \quad (28)$$

The components corresponding to transitions between operators in different irreducible chiral representations are consistent with $|Z_{nm}^{\overline{\text{MS}};Q}/Z_V^2| < 10^{-5}$ and thus set to zero in Eq. (28). The renormalization coefficients have been computed for the NPR operator basis (Eq. (14) in Ref. [52] using s quarks in place of d quarks. The results in Ref. [52] agree with Eq. (28) at the percent level, and deviations between the results are likely due to perturbative truncation errors, as Ref. [52] used nonperturbative step scaling [56,57]. The NPR basis renormalization coefficients are converted to the BSM basis using the change of

basis matrix, Eq. (15), and combined with the bare matrix elements to form renormalized matrix elements,

$$O_k(m_\pi, f_\pi, a, L) \equiv \langle \pi^+ | \mathcal{O}_k^{\overline{\text{MS}}}(\mathbf{p} = \mathbf{0}) | \pi^- \rangle(m_\pi, f_\pi, a, L). \quad (29)$$

On a given ensemble, the renormalization coefficients and bare matrix elements are computed on different configurations, as the former are only computed on a subset of ten of the configurations used to compute the matrix elements on each ensemble. As such, they are combined as an

TABLE II. Renormalized pion matrix elements $O_k(m_\pi, f_\pi, a, L)$, Eq. (29), of each operator \mathcal{O}_k in the BSM basis computed on each of the ensembles (upper), and the results of chiral continuum extrapolation (lower). The parameters α_k , β_k , and c_k are the χ EFT LECs, Eq. (30), and $\langle \pi^+ | \mathcal{O}_k^{\overline{\text{MS}}} | \pi^- \rangle$ is the extrapolated matrix element in the continuum and infinite volume limit at physical quark masses in the $\overline{\text{MS}}$ scheme at $\mu = 3$ GeV.

Operator		\mathcal{O}_1	\mathcal{O}_2	\mathcal{O}_3	$\mathcal{O}_{1'}$	$\mathcal{O}_{2'}$
Ensemble	am_ℓ	$O_k(m_\pi, f_\pi, a, L)$				
24I	0.01	-0.0190(11)	-0.0467(15)	0.001602(59)	-0.0850(32)	0.01556(50)
	0.005	-0.0162(11)	-0.0391(15)	0.000815(28)	-0.0733(32)	0.01305(45)
32I	0.008	-0.0204(15)	-0.0436(18)	0.001383(57)	-0.0863(39)	0.01393(66)
	0.006	-0.0179(13)	-0.0387(14)	0.000937(39)	-0.0771(36)	0.01239(50)
	0.004	-0.0160(15)	-0.0347(16)	0.000569(24)	-0.0696(37)	0.01115(60)
Extrapolated $O_k(m_\pi^{(\text{phys})}, f_\pi^{(\text{phys})}, 0, \infty)$						
$\langle \pi^+ \mathcal{O}_k^{\overline{\text{MS}}} \pi^- \rangle$ (GeV ⁴)		-0.0127(16)	-0.0245(22)	0.0000869(80)	-0.0535(48)	0.00757(75)
β_k		-1.21(17)	-2.37(23)	0.606(66)	-5.17(51)	0.735(80)
α_k (fm ⁻²)		-0.27(31)	0.33(23)	0.13(22)	-0.04(23)	0.58(26)
c_k		-0.6(1.4)	-1.17(98)	8.6(1.4)	-1.18(98)	-1.5(1.0)
χ^2/dof		0.02	0.03	0.22	0.08	0.03

uncorrelated product and their errors are added in quadrature. The renormalized matrix elements are shown in Table II.

III. CHIRAL EXTRAPOLATION

The renormalized matrix elements $O_k(m_\pi, f_\pi, a, L)$, Eq. (29), computed on each ensemble, are extrapolated to the continuum and infinite volume limit and physical pion mass using χ EFT at NLO; the relevant expressions have been derived in Ref. [37] using the Lagrangian in Eq. (4). The chiral models \mathcal{F}_k for O_k are given by

$$\begin{aligned}
&\mathcal{F}_1(m_\pi, f_\pi, a, L; \alpha_1, \beta_1, c_1) \\
&= \frac{\beta_1 \Lambda_\chi^4}{(4\pi)^2} \left[1 + \epsilon_\pi^2 (\log \epsilon_\pi^2 - 1 + c_1 - f_0(m_\pi L)) \right. \\
&\quad \left. + 2f_1(m_\pi L) + \alpha_1 a^2 \right], \\
&\mathcal{F}_2(m_\pi, f_\pi, a, L; \alpha_2, \beta_2, c_2) \\
&= \frac{\beta_2 \Lambda_\chi^4}{(4\pi)^2} \left[1 + \epsilon_\pi^2 (\log \epsilon_\pi^2 - 1 + c_2 - f_0(m_\pi L)) \right. \\
&\quad \left. + 2f_1(m_\pi L) + \alpha_2 a^2 \right], \\
&\mathcal{F}_3(m_\pi, f_\pi, a, L; \alpha_3, \beta_3, c_3) \\
&= \epsilon_\pi^2 \frac{\beta_3 \Lambda_\chi^4}{(4\pi)^2} \left[1 - \epsilon_\pi^2 (3 \log \epsilon_\pi^2 + 1 - c_3 + f_0(m_\pi L)) \right. \\
&\quad \left. + 2f_1(m_\pi L) + \alpha_3 a^2 \right], \tag{30}
\end{aligned}$$

where $\epsilon_\pi^2 = m_\pi^2/\Lambda_\chi^2$ is a power-counting parameter for χ EFT, β_k are the LO LECs defined in Eq. (4), and α_k and c_k are the additional NLO LECs. The matrix elements $O_{1'}$ and $O_{2'}$ have the same chiral behavior as O_1 and O_2 and are modeled by \mathcal{F}_1 and \mathcal{F}_2 , respectively, but with different LECs, $\alpha_{1'}$, $\beta_{1'}$, $c_{1'}$ and $\alpha_{2'}$, $\beta_{2'}$, $c_{2'}$. The functions

$$\begin{aligned}
f_0(mL) &= -2 \sum_{|n| \neq 0} K_0(mL|n|), \\
f_1(mL) &= 4 \sum_{|n| \neq 0} \frac{K_1(mL|n|)}{mL|n|} \tag{31}
\end{aligned}$$

are sums of modified Bessel functions $K_i(z)$ arising from one-loop, finite volume χ EFT in the p regime.

The models are fit to the data in Table II, using least-squares minimization including the correlations between O_k , m_π , and f_π on each ensemble. The final extrapolated results for the matrix elements and corresponding LECs are given in Table II. The resulting fits are shown in Fig. 4, where to isolate the pion-mass dependence of the matrix elements, ϵ_π^2 has been rescaled by $(f_\pi^{(\text{lat})}/f_\pi^{(\text{phys})})^2$ and the values of $O_k(m_\pi, f_\pi, a, L)$ have been shifted by $-\mathcal{F}_k(m_\pi, f_\pi, a, L; \alpha_k, \beta_k, c_k) + \mathcal{F}_k(m_\pi, f_\pi^{(\text{phys})}, 0, \infty; \alpha_k, \beta_k, c_k)$, where α_k , β_k , c_k are the best-fit coefficients given in Table II. The extrapolation bands for each O_k depict the functional form $\mathcal{F}_k(m_\pi, f_\pi^{(\text{phys})}, 0, \infty; \alpha_k, \beta_k, c_k)$. The results for $\langle \pi^+ | \mathcal{O}_k^{\overline{\text{MS}}} | \pi^- \rangle$ obey the same hierarchy as the chiral $SU(3)$ estimates [36] and are consistent with these results within 2 standard deviations.

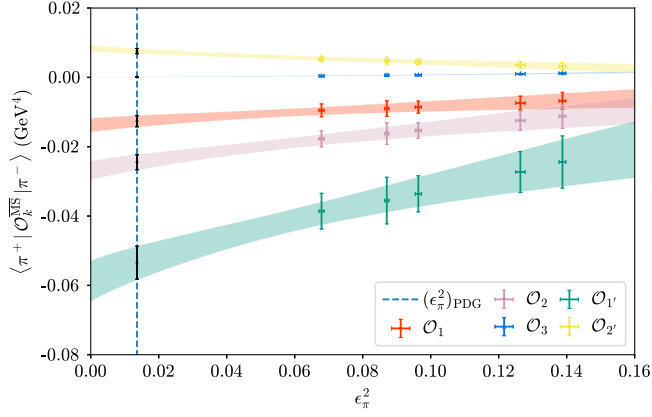


FIG. 4. Chiral extrapolation of renormalized matrix elements. The LQCD results are shown at $\epsilon_\pi^2 = m_\pi^2/(8\pi^2 f_\pi^2)$ calculated using the pion mass of each ensemble and the physical value of f_π , and the values of $\mathcal{O}_k(m_\pi, f_\pi, a, L)$ have been shifted by $-\mathcal{F}_k(m_\pi, f_\pi, a, L; \alpha_k, \beta_k, c_k) + \mathcal{F}_k(m_\pi, f_\pi^{(\text{phys})}, 0, \infty; \alpha_k, \beta_k, c_k)$, where α_k, β_k, c_k are the best-fit coefficients given in Table II. The physical pion mass is denoted by the dashed line.

The results for the renormalized, extrapolated, matrix elements differ from the results of Ref. [37] by about 2.0 to 5.0 standard deviations. There are a number of differences between the two calculations which may account for the discrepancy. The present calculation was performed with the same domain-wall action for the valence and sea quarks and is thus unitary, while that of Ref. [37] used a mixed action where unitarity is only restored in the continuum limit. Using the domain-wall action for valence and sea quarks yields matrix elements that have a mild dependence on the lattice spacing. In contrast, the mixed action results appear to have a larger dependence on the lattice spacing. However, the analysis of Ref. [37] was performed on nine ensembles with pion masses $m_\pi \lesssim 310$ MeV, including one ensemble with pion mass below the physical point, which allows for an interpolation to the physical point. Reference [37] also uses three lattice spacings as opposed to the two used in this computation, which allows for higher control of discretization artifacts in the non-perturbative renormalization and the chiral and continuum extrapolation.

IV. CONCLUSION

This work presents a determination of the renormalized matrix elements and χ EFT LECs for the short-distance operators that potentially arise from BSM physics at high scales and are relevant for the $\pi^- \rightarrow \pi^+ e^- e^-$ transition. The present calculation is the first to use chiral fermions with the same valence and sea quark actions. The domain-wall action yields a simple renormalization coefficient structure and straightforward extrapolation to the continuum and infinite volume limit and physical value of the light quark mass. With the results of Ref. [34], this completes the

calculation of both the long- and short-distance amplitudes for $\pi^- \rightarrow \pi^+ e^- e^-$ on the same gauge-field ensembles.

One may compare the relative size of the decay amplitude of $\pi^- \rightarrow \pi^+ e^- e^-$ induced by short-distance mechanisms, \mathcal{A}_{SD} , to that induced by long-distance mechanisms, \mathcal{A}_{LD} . In any model with a seesaw-type mechanism [59], for example the minimal left-right symmetric model [22], the effective Majorana neutrino mass $m_{\beta\beta}$ scales as $c/(G_F \Lambda_{\text{LNV}})$, where c is a Wilson coefficient. This implies

$$\begin{aligned} \frac{\mathcal{A}_{\text{SD}}}{\mathcal{A}_{\text{LD}}} &= \frac{G_F^2}{\Lambda_{\text{LNV}}^2} \frac{|\sum_k c_k \langle \pi^+ | \mathcal{O}_k | \pi^- \rangle|}{G_F^2 m_{\beta\beta} |M^{0\nu}|} \\ &= G_F \frac{|\sum_k c_k \langle \pi^+ | \mathcal{O}_k | \pi^- \rangle|}{c |M^{0\nu}|} \\ &\sim G_F \frac{\Lambda_{\text{QCD}}^4}{\Lambda_{\text{QCD}}^2} \sim 10^{-5}, \end{aligned} \quad (32)$$

where $M^{0\nu}$ is the long-distance nuclear matrix element for $\pi^- \rightarrow \pi^+ e^- e^-$. The final line of Eq. (32) arises by assuming that in a given BSM model, the dimensionless Wilson coefficients, c_k and c , describing each amplitude are order 1, and by using dimensional arguments to approximate the matrix elements. In particular, the long-distance nuclear matrix element includes the convolution of a massless bosonic propagator with a bilocal QCD matrix element. The convolution picks out the dimensional scale $1/\Lambda_{\text{QCD}}^2$, thereby enhancing the long-distance contribution compared to the short-distance one.

Since $\langle \pi^+ | \mathcal{O}_k | \pi^- \rangle$ and $M^{0\nu}$ have now been computed consistently in LQCD, it is possible to compute the ratio of Eq. (32), quantitatively, given the Wilson coefficients c_k and c from some model. For example, taking $c_k = c = 1$, and using the LQCD results from this work and of Ref. [34] for the matrix elements yields $\frac{\mathcal{A}_{\text{SD}}}{\mathcal{A}_{\text{LD}}} = 6.1(2) \times 10^{-5}$, consistent with expectations.

In addition to the pion-pion χ EFT LECs, the other LECs contributing to nuclear $0\nu\beta\beta$ decay must be determined in future calculations in order to constrain models of new physics from experimental constraints on nuclear $0\nu\beta\beta$ decay rates. Knowledge of these LECs may be used as input for models of nuclear many-body physics, which may be used to estimate the half-lives of various nuclear $0\nu\beta\beta$ decay processes from short-distance mechanisms with increasing precision. The other LO LECs that are necessary for describing nuclear $0\nu\beta\beta$ decay are from the nucleon-nucleon interaction [Fig. 1(b)], and may be determined with knowledge of the $\langle p^+ p^+ | \mathcal{O}_k(\mathbf{p} = \mathbf{0}) | n^0 n^0 \rangle$ matrix elements [33]. Calculations of these matrix elements are ongoing and will provide the first direct LQCD probe of $0\nu\beta\beta$ decay in nuclear systems.

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Furthermore, the TIKZ-FEYNMAN package [67] was used to generate diagrams for this manuscript, and the RunDec3 package [68] was used to run the strong coupling in the perturbative matching for the renormalization. This work is supported in part by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under Grant Contract No. DE-SC0011090. W.D. is also supported by the SciDAC5 Award No. DE-SC0023116. P.E.S. is additionally supported by the National Science Foundation under EAGER Grant No. 2035015, and by the U.S. DOE Early Career Award No. DE-SC0021006.

APPENDIX A: THREE-POINT CONTRACTIONS

The correlation functions of Eq. (6) can be written in terms of the following contraction structures:

$$\begin{aligned}
\textcircled{1}_{\Gamma_1\Gamma_2} &= \sum_x \text{Tr}[\gamma_5\Gamma_1 S_d(t_- \rightarrow x) S_u^\dagger(t_- \rightarrow x)] \cdot \text{Tr}[\gamma_5\Gamma_2 S_d(t_+ \rightarrow x) S_u^\dagger(t_+ \rightarrow x)] + (t_- \leftrightarrow t_+), \\
\textcircled{2}_{\Gamma_1\Gamma_2} &= \sum_x \text{Tr}[\gamma_5\Gamma_1 S_d(t_- \rightarrow x) S_u^\dagger(t_- \rightarrow x) \gamma_5\Gamma_2 S_d(t_+ \rightarrow x) S_u^\dagger(t_+ \rightarrow x)] + (t_- \leftrightarrow t_+), \\
\textcircled{3}_{\Gamma_1\Gamma_2} &= \sum_x \text{Tr}_D[\text{Tr}_D[\gamma_5\Gamma_1 S_d(t_- \rightarrow x) S_u^\dagger(t_- \rightarrow x)] \cdot \text{Tr}_D[\gamma_5\Gamma_2 S_d(t_+ \rightarrow x) S_u^\dagger(t_+ \rightarrow x)]] + (t_- \leftrightarrow t_+), \\
\textcircled{4}_{\Gamma_1\Gamma_2} &= \sum_x \text{Tr}_D[\text{Tr}_C[\gamma_5\Gamma_1 S_d(t_- \rightarrow x) S_u^\dagger(t_- \rightarrow x)] \cdot \text{Tr}_C[\gamma_5\Gamma_2 S_d(t_+ \rightarrow x) S_u^\dagger(t_+ \rightarrow x)]] + (t_- \leftrightarrow t_+), \tag{A1}
\end{aligned}$$

where Γ_1, Γ_2 are arbitrary Dirac matrices, Tr_C (Tr_D) denotes a color (spin) trace, $\text{Tr} = \text{Tr}_C \circ \text{Tr}_D$ denotes a full trace, and $x = (\mathbf{x}, t_x)$. Propagators $S(t_{\text{src}} \rightarrow x)$ are computed with a zero three-momentum wall source at time $t_{\text{src}} \in \{t_-, t_+\}$ and a point sink at time t_x ,

$$S(t_{\text{src}} \rightarrow x) \equiv \sum_y S((\mathbf{y}, t_{\text{src}}) \rightarrow (\mathbf{x}, t_x)). \tag{A2}$$

With the definitions of Eq. (A1), the correlation functions are evaluated as

$$\begin{aligned}
\mathcal{C}_1(t_-, t_x, t_+) &= -\frac{1}{4} [\textcircled{1}_{VV} - \textcircled{2}_{VV} - \textcircled{1}_{AV} + \textcircled{2}_{AV} + \textcircled{1}_{VA} - \textcircled{2}_{VA} - \textcircled{1}_{AA} + \textcircled{2}_{AA}], \\
\mathcal{C}_2(t_-, t_x, t_+) &= -\frac{1}{2} [\textcircled{1}_{SS} - \textcircled{2}_{SS} + \textcircled{1}_{PP} - \textcircled{2}_{PP}], \\
\mathcal{C}_3(t_-, t_x, t_+) &= -\frac{1}{2} [\textcircled{1}_{VV} - \textcircled{2}_{VV} + \textcircled{1}_{AA} - \textcircled{2}_{AA}], \\
\mathcal{C}_1'(t_-, t_x, t_+) &= -\frac{1}{4} [\textcircled{3}_{VV} - \textcircled{4}_{VV} - \textcircled{3}_{AV} + \textcircled{4}_{AV} + \textcircled{3}_{VA} - \textcircled{4}_{VA} - \textcircled{3}_{AA} + \textcircled{4}_{AA}], \\
\mathcal{C}_2'(t_-, t_x, t_+) &= -\frac{1}{2} [\textcircled{3}_{SS} - 4\textcircled{4}_{SS} + \textcircled{3}_{PP} - \textcircled{4}_{PP}], \tag{A3}
\end{aligned}$$

where $S = 1$, $P = \gamma_5$, $V = \gamma^\mu$, and $A = \gamma^\mu \gamma_5$.

APPENDIX B: EFFECTIVE MATRIX ELEMENT FITS

Figures 5–8 display the remaining fits to the effective matrix elements [Eq. (8)] that were not depicted in Fig. 2. The fit procedure is described in Sec. II B of the main text. The number of gauge-field configurations per ensemble used in each matrix element extraction, n_{cfgs} , and the corresponding bare matrix elements in lattice units, Eq. (7), are shown in Table III.

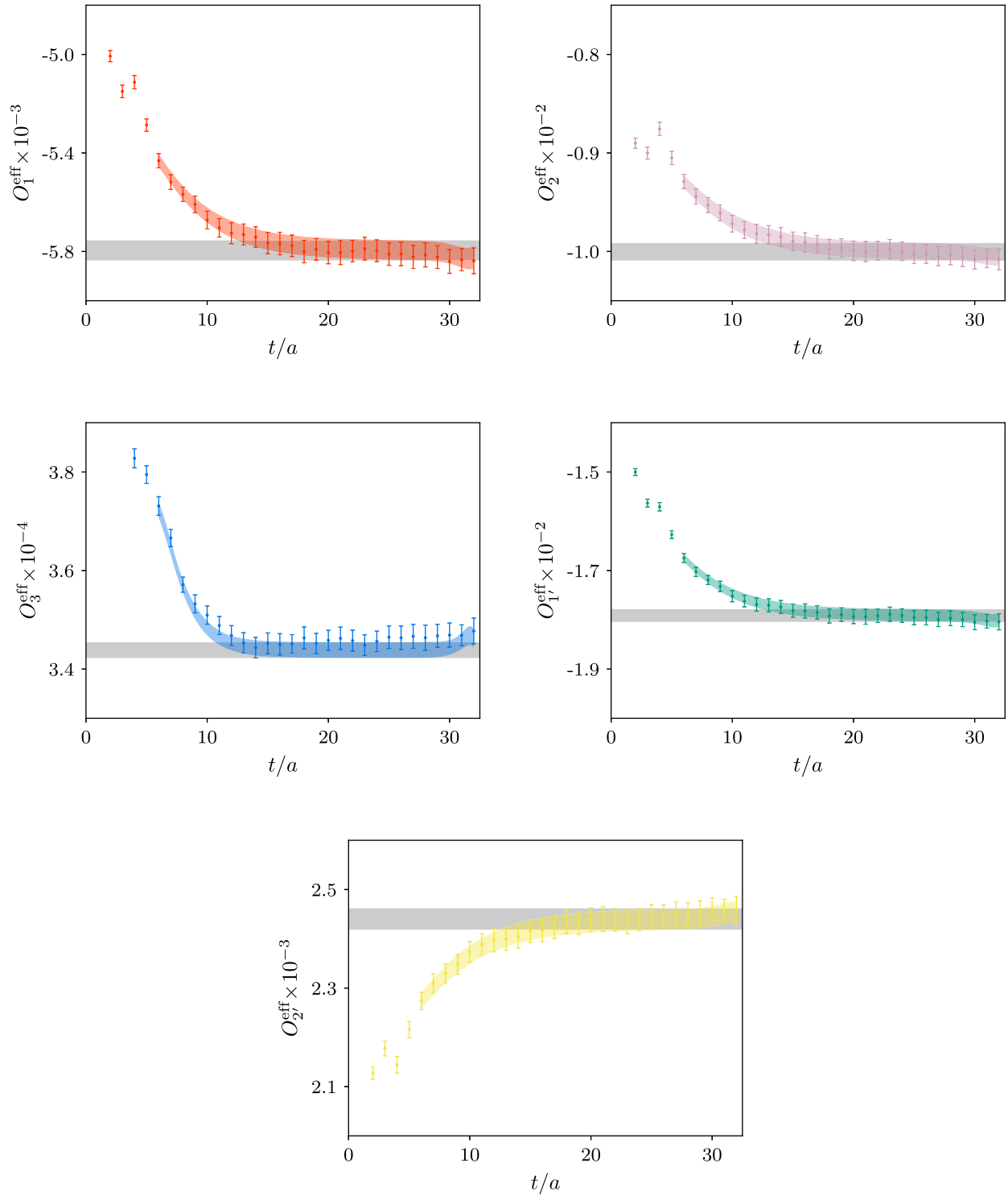


FIG. 5. Effective matrix elements, Eq. (8), for the operators $\mathcal{O}_k(\mathbf{p} = \mathbf{0})$ on the 24I, $am_\ell = 0.01$ ensemble. The constant gray band denotes the fit results for each bare, dimensionless matrix element $a^4 \langle \pi^+ | \mathcal{O}_k(\mathbf{p} = \mathbf{0}) | \pi^- \rangle$, and the colored data points and colored band denote the effective matrix element data and extrapolation band, respectively. The fit procedure is detailed in Sec. II B.

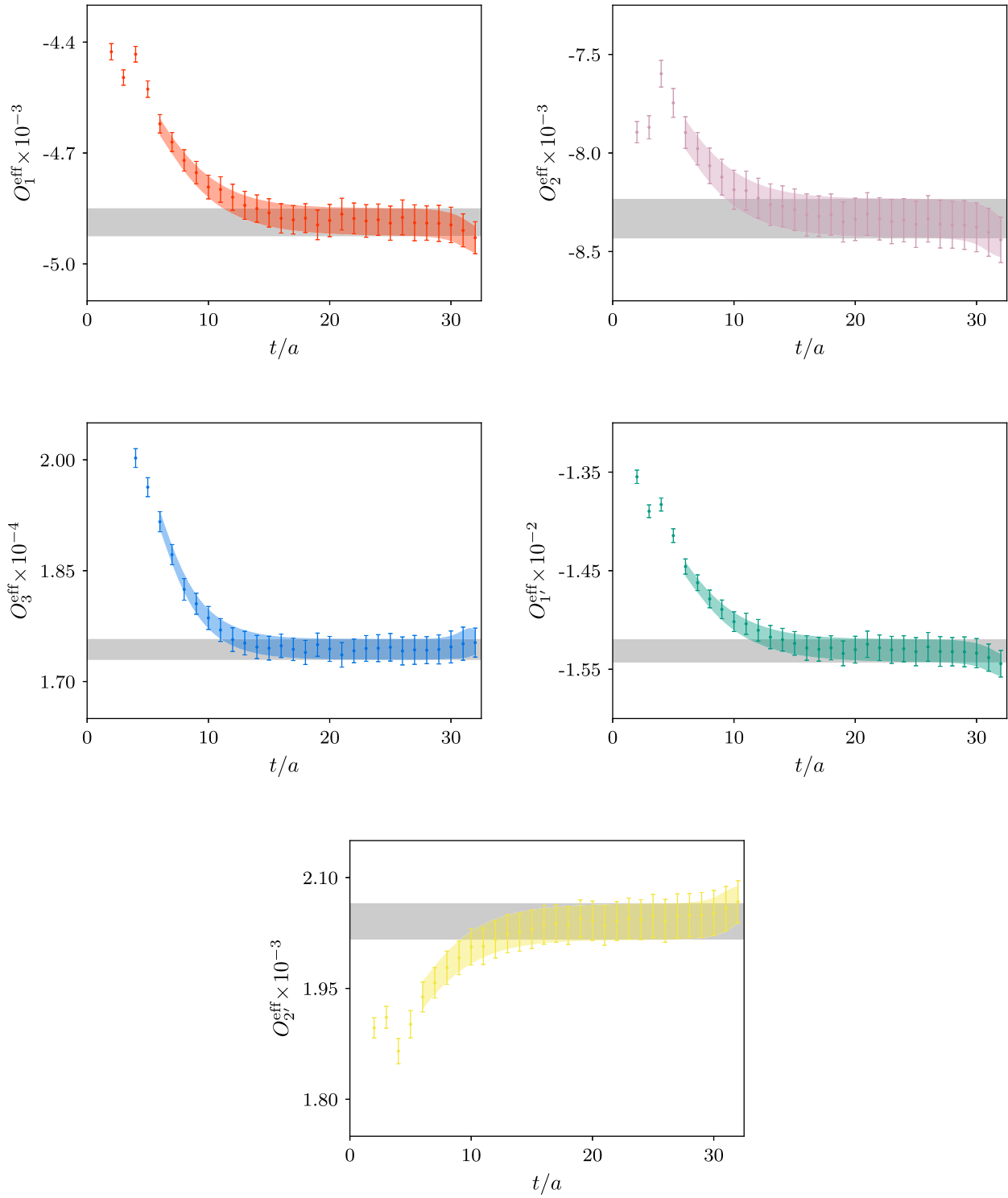


FIG. 6. As in Fig. 5, for the 24l, $am_\ell = 0.005$ ensemble.

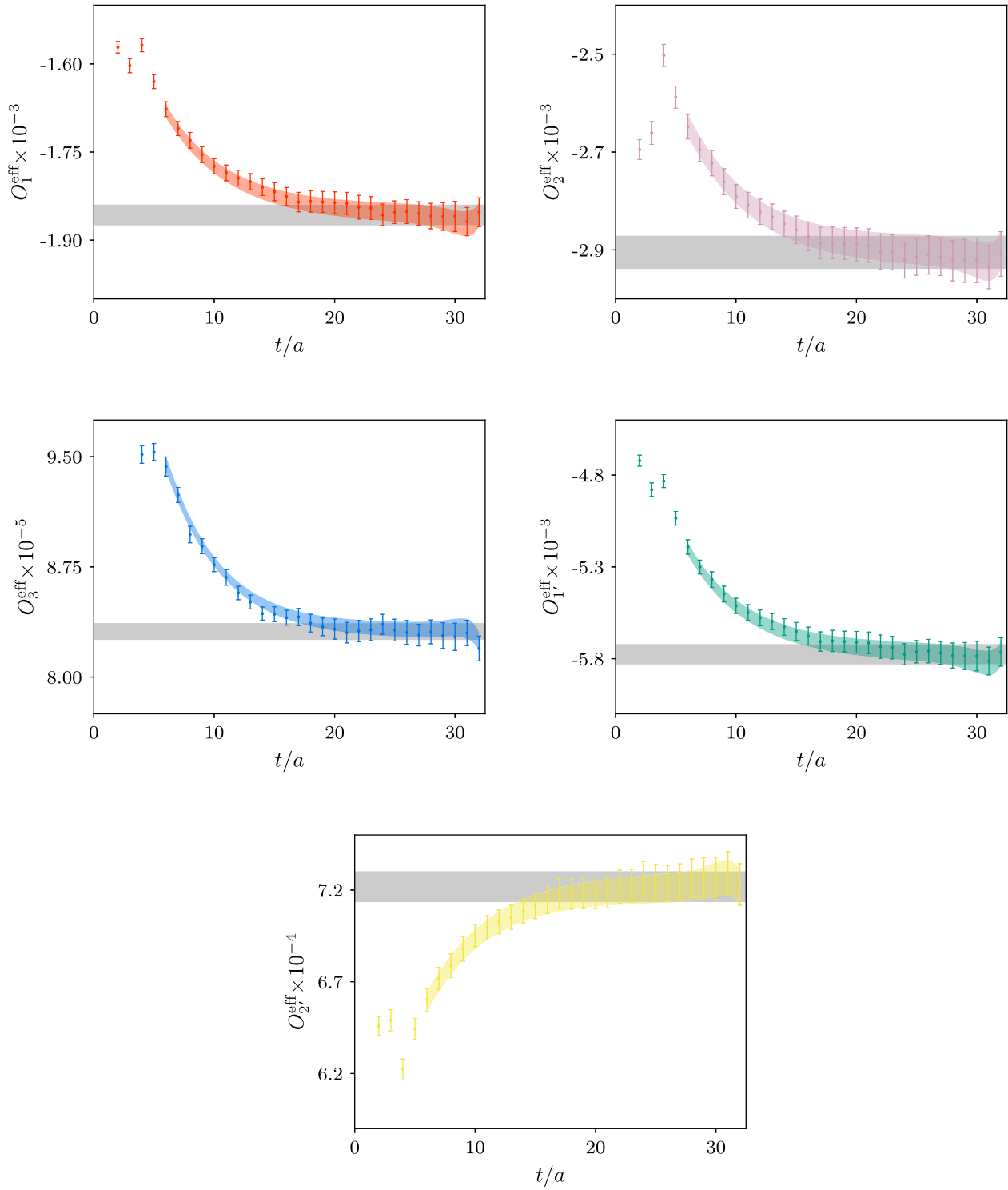


FIG. 7. As in Fig. 5, for the 32I, $am_\ell = 0.008$ ensemble.

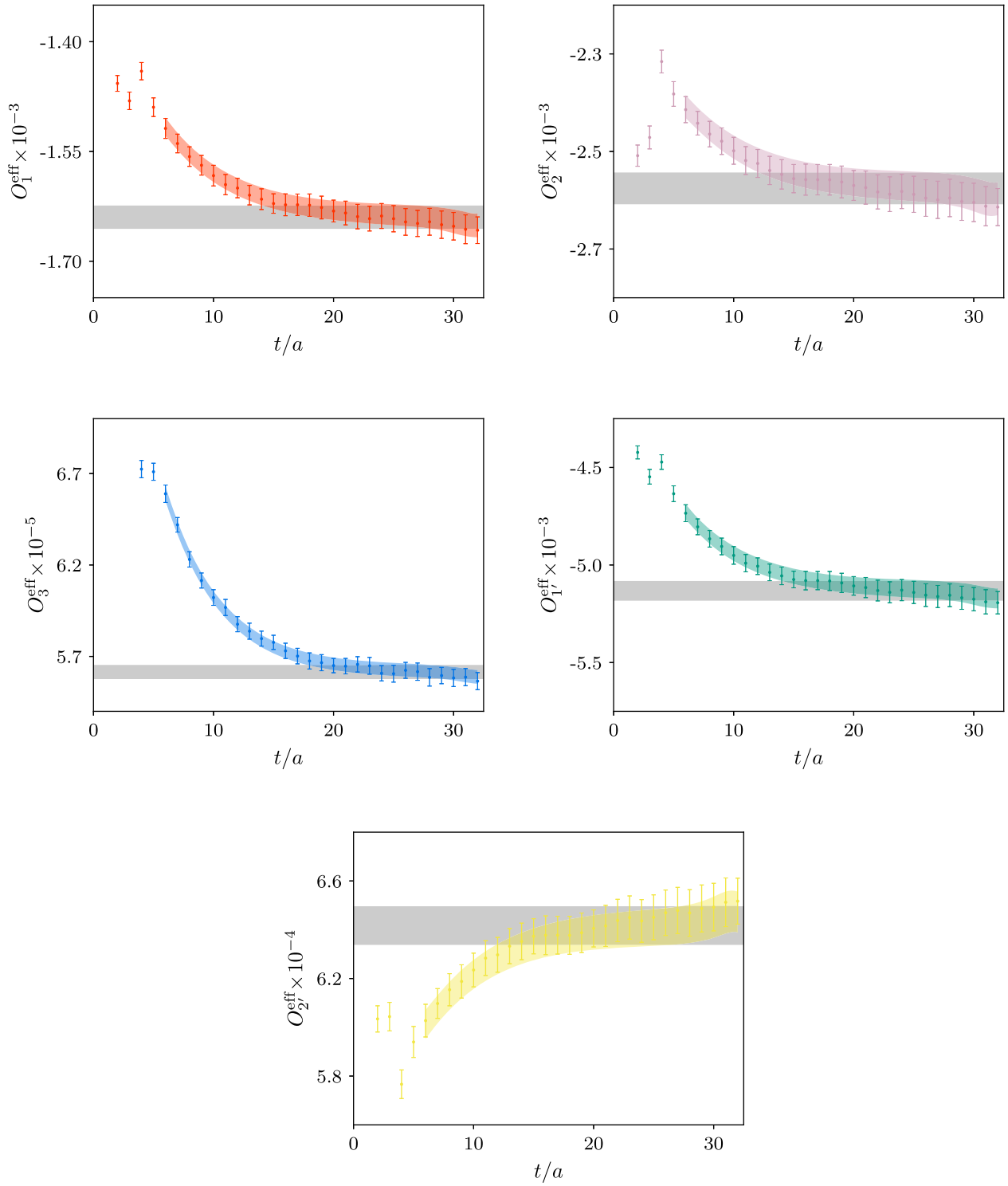


FIG. 8. As in Fig. 5, for the 32I, $am_\ell = 0.006$ ensemble.

TABLE III. Determination of bare matrix elements $a^4 \langle \pi^+ | \mathcal{O}_k | \pi^- \rangle$ on each ensemble for each operator $\mathcal{O}_k(x)$ in the BSM basis, Eq. (2), extracted from fits to the effective matrix elements [Eq. (8)] as described in the text. The effective matrix elements are computed on n_{cfgs} configurations on the respective ensemble.

Ensemble	am_ℓ	n_{cfgs}	$a^4 \langle \pi^+ \mathcal{O}_1 \pi^- \rangle$	$a^4 \langle \pi^+ \mathcal{O}_2 \pi^- \rangle$	$a^4 \langle \pi^+ \mathcal{O}_3 \pi^- \rangle$	$a^4 \langle \pi^+ \mathcal{O}_{1'} \pi^- \rangle$	$a^4 \langle \pi^+ \mathcal{O}_{2'} \pi^- \rangle$
24I	0.01	52	-0.005804(41)	-0.010023(91)	0.0003442(16)	-0.01794(13)	0.002445(22)
	0.005	53	-0.004891(38)	-0.00834(11)	0.0001742(14)	-0.01533(12)	0.002043(26)
32I	0.008	33	-0.001862(17)	-0.002917(34)	0.00008286(58)	-0.005791(53)	0.0007248(86)
	0.006	42	-0.001644(16)	-0.002587(36)	0.00005600(40)	-0.005145(50)	0.0006445(87)
	0.004	47	-0.001482(15)	-0.002331(31)	0.00003391(40)	-0.004669(47)	0.0005822(78)

APPENDIX C: VECTOR AND AXIAL-VECTOR RENORMALIZATION COEFFICIENTS

Calculation of the scale and scheme-independent vector and axial-vector-current renormalization coefficients $\mathcal{Z}_j(a)$, with $j \in \{V, A\}$, proceeds through the vector [Eq. (23)] and axial-vector three-point functions,

$$G_A^\mu(q; a, m_\ell) = \frac{1}{V} \sum_{x, x_1, x_2} e^{i(p_1 \cdot x_1 - p_2 \cdot x_2 + q \cdot x)} \langle 0 | u(x_1) A^\mu(x) \bar{d}(x_2) | 0 \rangle, \quad (\text{C1})$$

where $A^\mu(x) = \bar{u}(x) \gamma^\mu \gamma_5 d(x)$. The momenta p_1 , p_2 , and q are subject to the symmetric constraint, Eq. (17), and

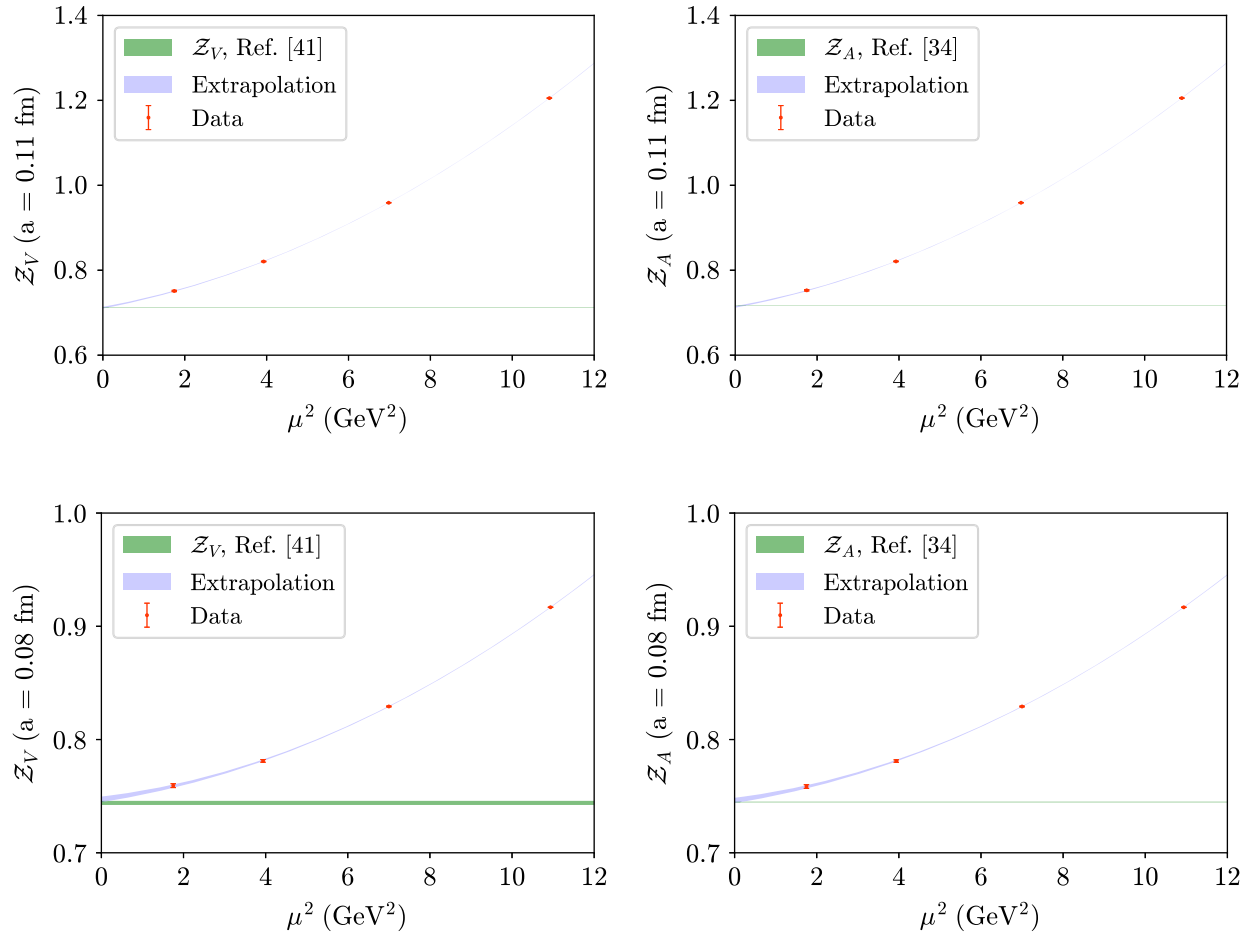


FIG. 9. Vector and axial-vector renormalization coefficients computed by the procedure described in the text, and extrapolated to $\mu^2 = 0$ with the model given in Eq. (C5). The red data points are the computed data, Eq. (C3), the blue bands show the extrapolation to $\mu^2 \rightarrow 0$, and the green bands denote the chiral limit value of \mathcal{Z}_A and \mathcal{Z}_V computed in Refs. [34,48].

parametrized identically to the modes used in the calculation of the four-quark operator renormalizations [Eq. (18)] with $k \in \{2, 3, 4, 5\}$. The lattice spacing dependence is made explicit in this section. The amputated three-point functions

$$\Lambda_j^\mu(q; a, m_\ell) = S^{-1}(p_1; a, m_\ell) G_j^\mu(q; a, m_\ell) S^{-1}(p_2; a, m_\ell), \quad (\text{C2})$$

with $j \in \{V, A\}$, are used to compute the renormalization coefficients,

$$\begin{aligned} \frac{1}{12\tilde{q}^2} \frac{\mathcal{Z}_V(\mu^2; a, m_\ell)}{\mathcal{Z}_q^{\text{RI/sMOM}}(\mu^2; a, m_\ell)} \text{Tr}[\tilde{q}_\mu \Lambda_V^\mu(q; a, m_\ell) \tilde{q}] \Big|_{\text{sym}} &= 1, \\ \frac{1}{12\tilde{q}^2} \frac{\mathcal{Z}_A(\mu^2; a, m_\ell)}{\mathcal{Z}_q^{\text{RI/sMOM}}(\mu^2; a, m_\ell)} \text{Tr}[\tilde{q}_\mu \Lambda_A^\mu(q; a, m_\ell) \gamma_5 \tilde{q}] \Big|_{\text{sym}} &= 1, \end{aligned} \quad (\text{C3})$$

where $\tilde{p}_\mu = \frac{2}{a} \sin(\frac{a}{2} p_\mu)$ is the lattice momentum. Note that the quark-field renormalization in Eq. (C3) is defined in the RI/sMOM scheme [51],

$$\begin{aligned} \mathcal{Z}_q^{\text{RI/sMOM}}(\mu^2; a, m_\ell) \Big|_{p^2=\mu^2} \\ = \frac{i}{12\tilde{p}^2} \text{Tr} \left[S^{-1}(p; a, m_\ell) \tilde{p} \right] \Big|_{p^2=\mu^2}, \end{aligned} \quad (\text{C4})$$

which differs from the RI γ scheme [52] of Eq. (22); \mathcal{Z}_V and \mathcal{Z}_A are scheme independent, and hence may be computed in any scheme. The chiral limits $\mathcal{Z}_V(\mu^2; a)$ and $\mathcal{Z}_A(\mu^2; a)$ of $\mathcal{Z}_V(\mu^2; a, m_\ell)$ and $\mathcal{Z}_A(\mu^2; a, m_\ell)$ are evaluated by a joint, correlated linear extrapolation of $\{\mathcal{Z}_q^{\text{RI/sMOM}}, \mathcal{Z}_V, \mathcal{Z}_A\}$ in m_ℓ , identical to the procedure used in the $am_\ell \rightarrow 0$ extrapolation of $\{\mathcal{Z}_q^{\text{RI}\gamma}/\mathcal{Z}_V, F_{nm}\}$, as described in Sec. II C of the text [Eqs. (21)–(24)].

Although the renormalization coefficients $\mathcal{Z}_V, \mathcal{Z}_A$ are scale independent, the RI procedure introduces scale dependence from the kinematic setup [Eq. (17)]. This scale dependence is removed by fitting $\mathcal{Z}_j(\mu^2; a)$ to a power series in μ^2 and taking the $\mu^2 \rightarrow 0$ limit as described

in Ref. [69], with fit model:

$$\mathcal{Z}_j(\mu^2; a) = \mathcal{Z}_j(a) + c_j^{(1)}(a)\mu^2 + c_j^{(2)}(a)\mu^4. \quad (\text{C5})$$

Here $\mathcal{Z}_j(a)$, $c_j^{(1)}(a)$, and $c_j^{(2)}(a)$ are coefficients which are determined by correlated χ^2 minimization. The fits are shown in Fig. 9. The fits have χ^2/dof ranging between 0.15 and 0.71. The best-fit value of $\mathcal{Z}_j(a)$ is the value that is taken for the renormalization factor, and it is determined that

$$\begin{aligned} \mathcal{Z}_V(0.11 \text{ fm}) &= 0.7119(20), & \mathcal{Z}_V(0.08 \text{ fm}) &= 0.7472(24), \\ \mathcal{Z}_A(0.11 \text{ fm}) &= 0.7137(19), & \mathcal{Z}_A(0.08 \text{ fm}) &= 0.7462(23). \end{aligned} \quad (\text{C6})$$

The results show that $\mathcal{Z}_V = \mathcal{Z}_A$ within statistical precision as expected. The determination presented in this work is consistent with the determination of \mathcal{Z}_V in Ref. [48] for the $a = 0.08$ fm and $a = 0.11$ fm ensembles, and with \mathcal{Z}_A in Ref. [34] for the $a = 0.08$ fm ensembles, although \mathcal{Z}_A differs from the $a = 0.11$ fm value in that work by about 1 standard deviation. This deviation may be due to discrepancies in the procedure used to extract \mathcal{Z}_A , as the fit model [Eq. (C5)] does not capture all the discretization artifacts present in the data.

APPENDIX D: RENORMALIZATION COEFFICIENT $am_\ell \rightarrow 0$ EXTRAPOLATION

Figures 10–17 display the $am_\ell \rightarrow 0$ extrapolations of $\mathcal{Z}_q^{\text{RI}\gamma}/\mathcal{Z}_V$ and F_{nm} , as described in Sec. II C of the text. Each renormalization coefficient is evaluated at $q = \frac{2\pi}{L}(4, 4, 0, 0)$, which is the lattice momentum corresponding to the scale $\mu = \mu_4$. In each of Figs. 10–17, the q dependence of $(\mathcal{Z}_q^{\text{RI}\gamma}/\mathcal{Z}_V)(\mu^2; a)$ and the q dependence of $F_{nm}(q; a)$ has been suppressed for clarity. The data is observed to have very mild dependence on am_ℓ .

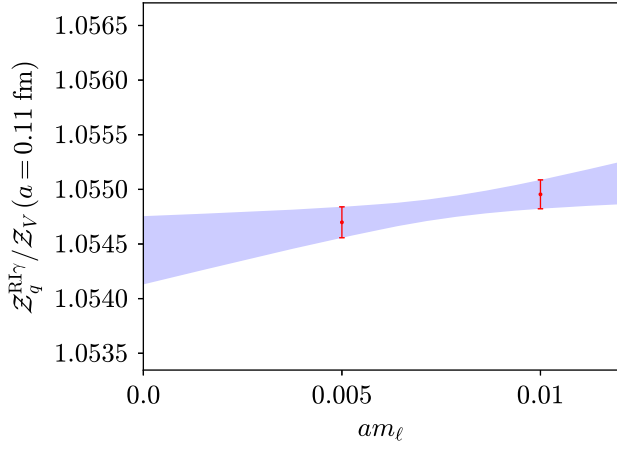


FIG. 10. The $am_\ell \rightarrow 0$ extrapolation for the RI quark-field renormalization $Z_q^{\text{RI}\gamma}/Z_V$, Eq. (22), computed on the $a = 0.11$ fm ensembles at $q = \frac{2\pi}{aL}(4, 4, 0, 0)$ and extrapolated to the chiral limit via a joint correlated linear extrapolation in am_ℓ [Eq. (24)]. The data is depicted in red and the shaded band denotes the extrapolation.

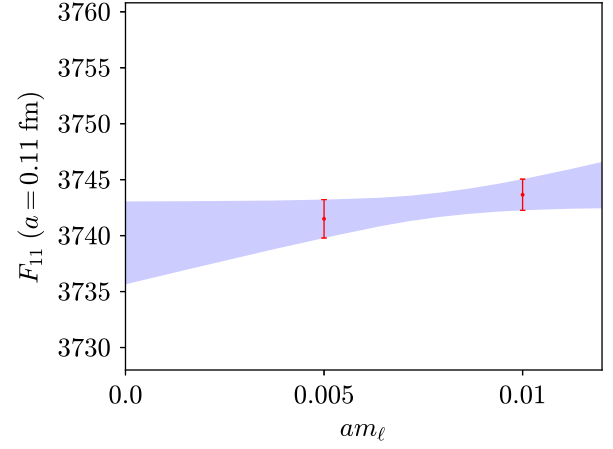


FIG. 11. As in Fig. 10, $am_\ell \rightarrow 0$ extrapolation for F_{nm} on the first irreducible chiral subspace $\{F_{11}\}$, for the $a = 0.11$ fm ensembles.

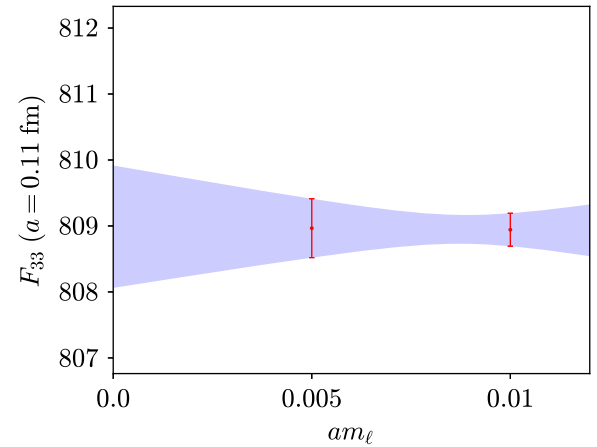
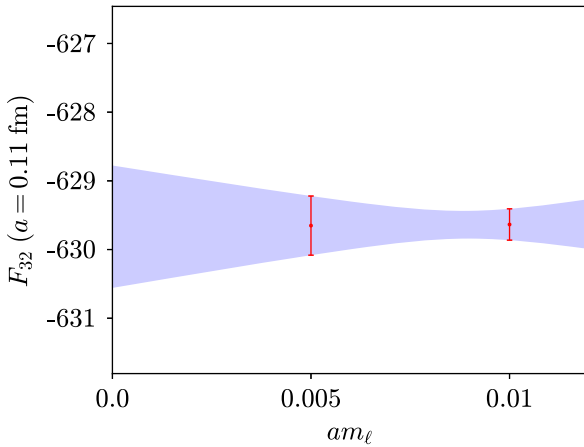
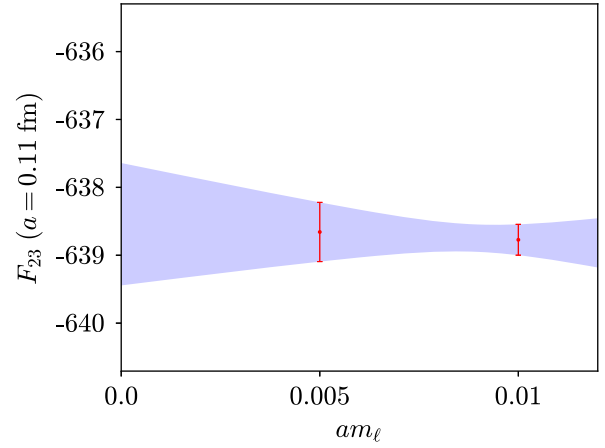
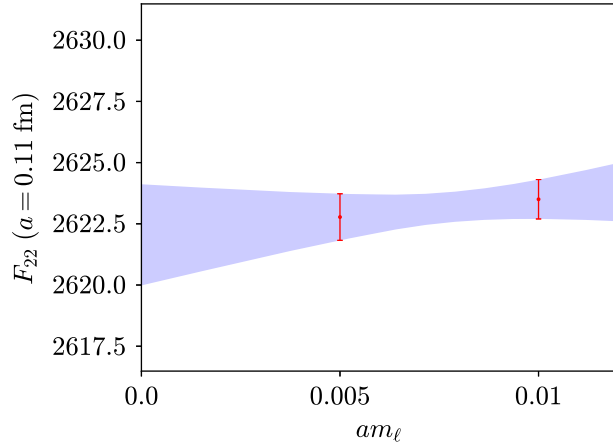


FIG. 12. As in Fig. 10, $am_\ell \rightarrow 0$ extrapolation for F_{nm} on the second irreducible chiral subspace $\{F_{22}, F_{23}, F_{32}, F_{33}\}$, for the $a = 0.11$ fm ensembles.

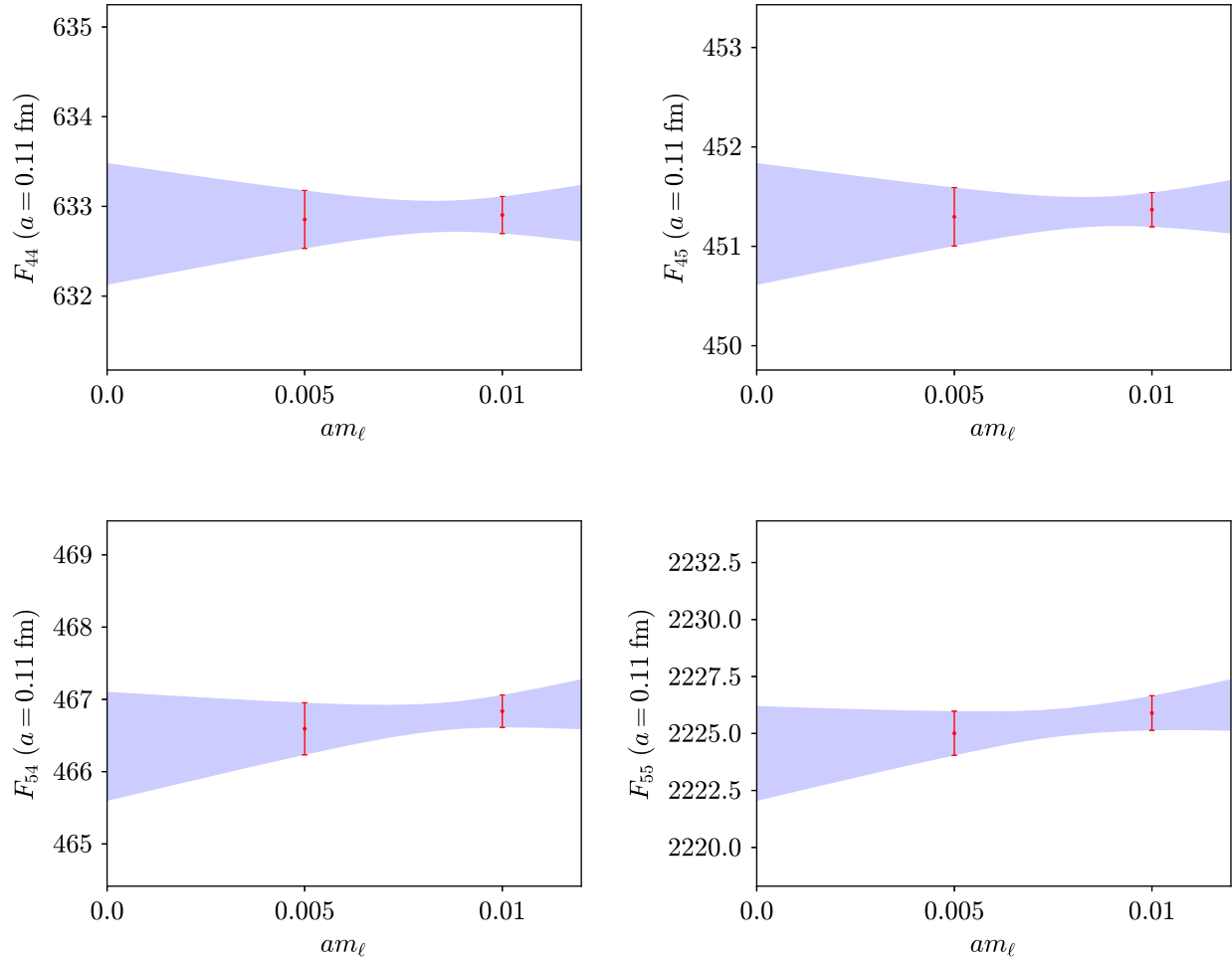


FIG. 13. As in Fig. 10, $am_\ell \rightarrow 0$ extrapolation for F_{nm} on the third irreducible chiral subspace $\{F_{44}, F_{45}, F_{54}, F_{55}\}$, for the $a = 0.11$ fm ensembles.

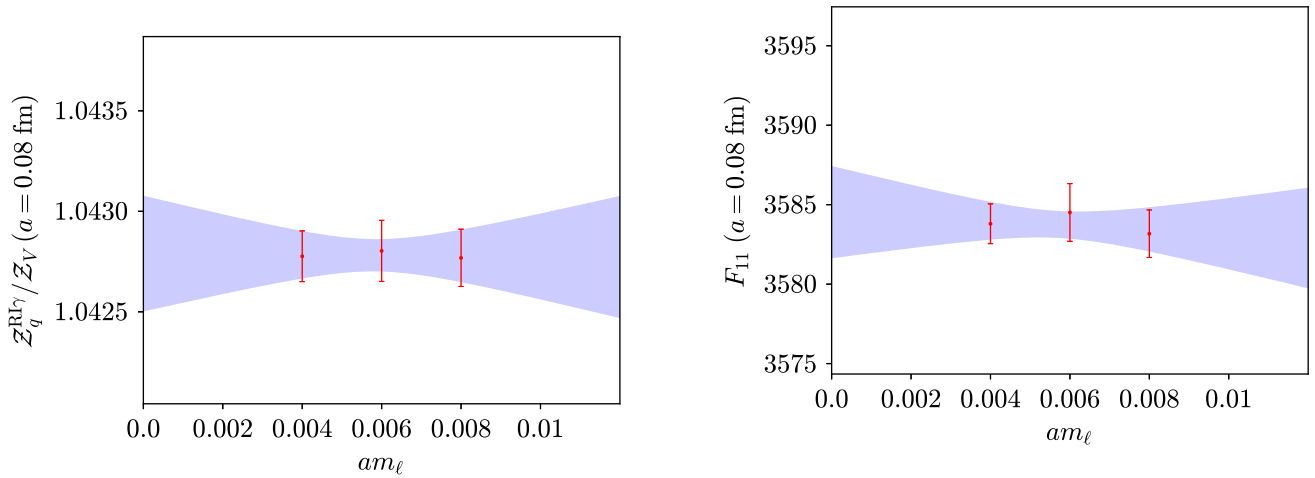


FIG. 14. As in Fig. 10, $am_\ell \rightarrow 0$ extrapolation for $Z_q^{\text{RI}\gamma} / Z_V$, for the $a = 0.08$ fm ensembles.

FIG. 15. As in Fig. 10, $am_\ell \rightarrow 0$ extrapolation for F_{nm} on the first irreducible chiral subspace $\{F_{11}\}$, for the $a = 0.08$ fm ensembles.

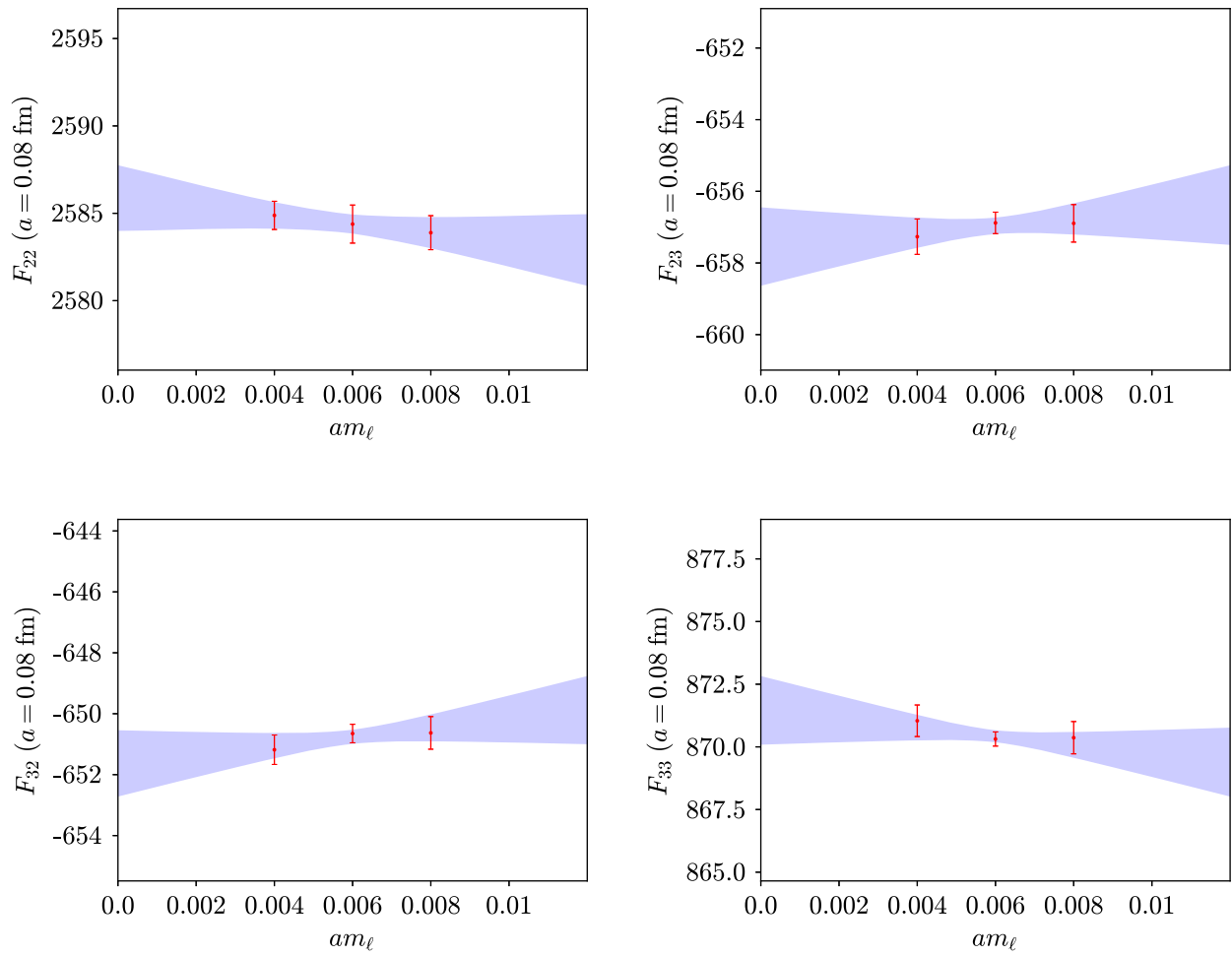


FIG. 16. As in Fig. 10, $am_\ell \rightarrow 0$ extrapolation for F_{nm} on the second irreducible chiral subspace $\{F_{22}, F_{23}, F_{32}, F_{33}\}$, for the $a = 0.08$ fm ensembles.

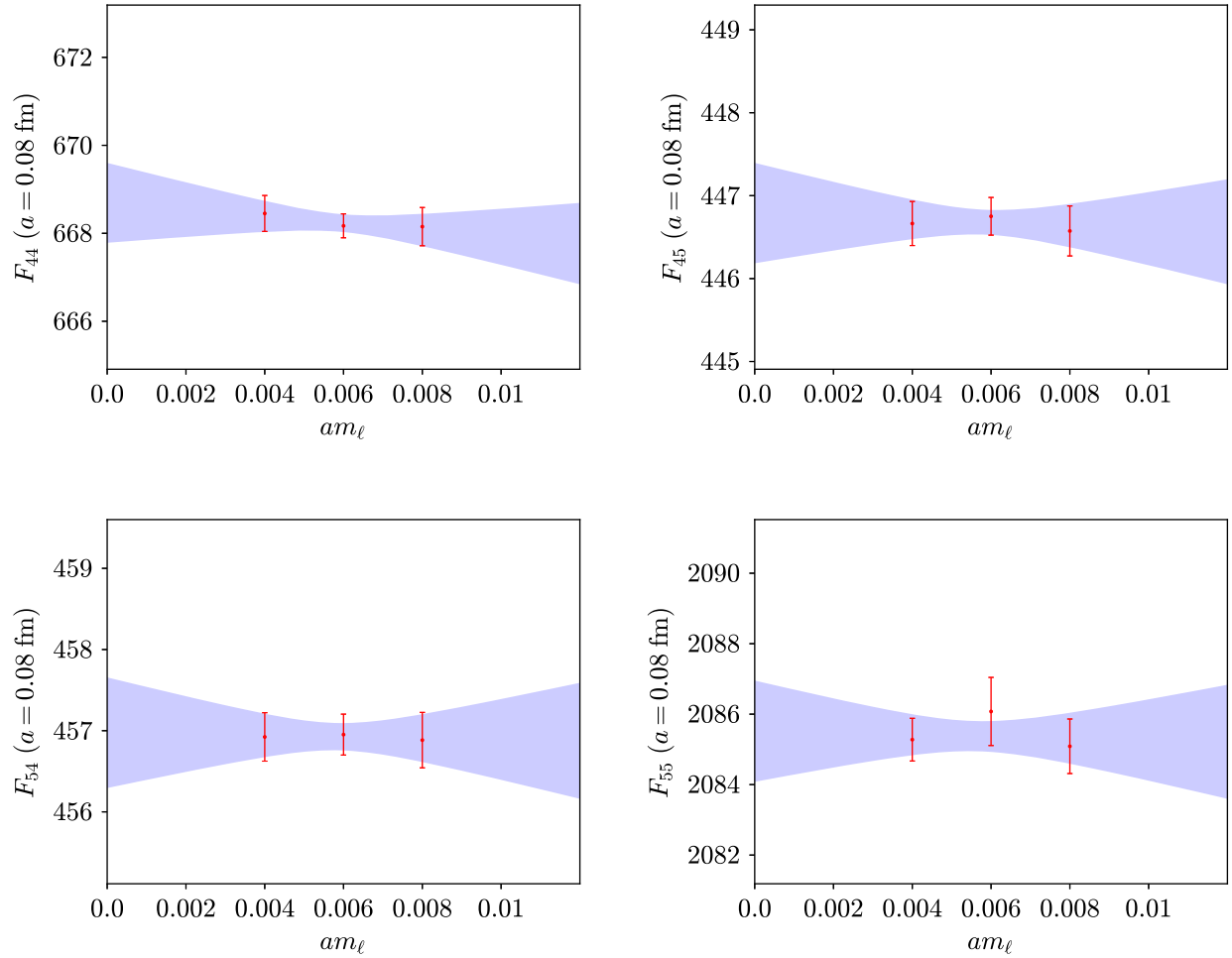


FIG. 17. As in Fig. 10, $am_\ell \rightarrow 0$ extrapolation for F_{nm} on the third irreducible chiral subspace $\{F_{44}, F_{45}, F_{54}, F_{55}\}$, for the $a = 0.08$ fm ensembles.

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