

Scalar size of the pion from lattice QCD

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We present a lattice QCD calculation of the pion scalar form factor and associated radii with fully controlled systematics. Lattice results are computed on a large set of 17 gauge ensembles with $N_f = 2 + 1$ Wilson Clover-improved sea quarks. These ensembles cover four values of the lattice spacing between $a = 0.049$ fm and $a = 0.086$ fm, a pion mass range of 130–350 MeV, and various physical volumes. A precise determination of the notorious quark-disconnected contributions facilitates an unprecedented momentum resolution for the form factor, particularly on large and fine ensembles in the vicinity of physical quark mass. A large range of source-sink separations $1.0 \text{ fm} \lesssim t_{\text{sep}} \lesssim 3.25 \text{ fm}$ is used to reliably extract the relevant ground state matrix elements at vanishing and nonvanishing momentum transfer. This allows us for the first time to obtain the scalar radii from a z -expansion parametrization of the Q^2 dependence of the resulting form factors rather than a simple, linear approximation at small momentum transfer. The physical extrapolation for the radii is carried out using three-flavor NLO chiral perturbation theory to parametrize the quark mass dependence in terms of three low-energy constants, including the first lattice determination of L_4^r . Systematic uncertainties on the final results related to the ground state extraction, form factor parametrization as well as the physical extrapolation are accounted for via model averages based on the Akaike information criterion. Our physical results for the pion singlet and octet scalar radii are $\langle r_S^2 \rangle_\pi^0 = 0.550(32)_{\text{stat}}(39)_{\text{sys}}[50]_{\text{total}} \text{ fm}^2$ and $\langle r_S^2 \rangle_\pi^8 = 0.443(16)_{\text{stat}}(45)_{\text{sys}}[47]_{\text{total}} \text{ fm}^2$, respectively. The values of the relevant low energy constants are given by $f_0 = 116.5(5.5)_{\text{stat}}(13.7)_{\text{sys}}[14.8]_{\text{total}} \text{ MeV}$, $L_4^r(\mu = 770 \text{ MeV}) = +0.38(09)_{\text{stat}}(15)_{\text{sys}}[18]_{\text{total}} \times 10^{-3}$ and $L_5^r(\mu = 770 \text{ MeV}) = +0.58(0.38)_{\text{stat}}(1.08)_{\text{sys}}[1.14]_{\text{total}} \times 10^{-3}$. For the light quark contribution to the pion scalar radius, we obtain $\langle r_S^2 \rangle_\pi^l = 0.515(28)_{\text{stat}}(32)_{\text{sys}}[43]_{\text{total}} \text{ fm}^2$, resulting in a value of $\bar{\epsilon}_4 = 3.99(15)_{\text{stat}}(17)_{\text{sys}}[23]_{\text{total}}$ for the pertinent low-energy constant in two-flavor chiral perturbation theory.

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I. INTRODUCTION

In the study of the strong interactions at low energies, quark-hadron duality dictates that there are essentially two different approaches that can be taken: either to describe the strong interactions on the phenomenological level of hadrons, such as is done in chiral perturbation theory (χ PT) and its various offshoots, or to rely on the fundamental quark and gluon degrees of freedom and to determine hadronic quantities nonperturbatively from the low-energy dynamics of quantum chromodynamics (QCD), such as by means of lattice QCD simulations.

With the advent of much improved algorithms and vastly increased computing power enabling large-scale simulations at physical quark masses, the working

relationship between lattice QCD and χ PT has changed: No longer is χ PT an essential tool required to extrapolate results from lattice simulations done at unphysically heavy quark masses to the physical point, but the ability of lattice simulations to vary the quark masses away from their physical values allows checking the validity of χ PT and extracting values for its low-energy constants (LECs).

Especially well suited for the latter purpose are quantities that depend only on one or two LECs, such as the scalar radii

$$\langle r_S^2 \rangle_\pi^f = - \frac{6}{F_S^{\pi,f}(0)} \left. \frac{dF_S^{\pi,f}(Q^2)}{dQ^2} \right|_{Q^2 \rightarrow 0} \quad (1)$$

parametrizing the slope of the scalar form factors ($Q^2 = -q^2 = -(p_f - p_i)^2$)

$$F_S^{\pi,f}(Q^2) = \langle \pi(\mathbf{p}_f) | \mathcal{S}^f | \pi(\mathbf{p}_i) \rangle, \quad (2)$$

where in the theory with $N_f = 2$ quark flavors, there is only one isoscalar scalar density

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$$S^I = \bar{u}u + \bar{d}d, \quad (3)$$

whereas for $N_f = 2 + 1$ quark flavors, the basic scalar densities are the singlet and octet ones,

$$S^0 = \bar{u}u + \bar{d}d - 2\bar{s}s, \quad (4)$$

$$S^8 = \bar{u}u + \bar{d}d + \bar{s}s. \quad (5)$$

We note that while the renormalization constants for the scalar densities are known [1], no renormalization is needed to extract the radii since the renormalization factors cancel in Eq. (1); we also note that there is no dimension-4 bilinear that could mix with the scalar densities, and hence, the scalar radii are automatically $O(a)$ improved.

In SU(2) χ PT, the scalar radius depends only on $\bar{\ell}_4$ via

$$\langle r_S^2 \rangle_\pi^I = \frac{1}{8\pi^2 f_{\pi,\text{phys}}^2} \left[-\frac{13}{2} + \bar{\ell}_4 + \log \frac{M_{\pi,\text{phys}}^2}{M_\pi^2} \right]. \quad (6)$$

In SU(3) χ PT, the scalar radii are related by [2]

$$\langle r_S^2 \rangle_\pi^0 = \langle r_S^2 \rangle_\pi^8 + \delta r_S^2, \quad (7)$$

$$\langle r_S^2 \rangle_\pi^I = \langle r_S^2 \rangle_\pi^8 + \frac{2}{3} \delta r_S^2, \quad (8)$$

where

$$\begin{aligned} \langle r_S^2 \rangle_\pi^8 = & \frac{1}{96\pi^2 f_0^2} \left[4608\pi^2 L_5^r - 60 - 2\frac{M_\pi^2}{M_\eta^2} + 18 \log \frac{M_K^2}{M_\pi^2} \right. \\ & \left. + \frac{45M_\pi^2 - 18M_K^2 - 27M_\eta^2}{M_K^2 - M_\pi^2} \log \frac{M_\pi^2}{\mu^2} \right], \end{aligned} \quad (9)$$

$$\delta r_S^2 = \frac{12}{f_0^2} \left[12L_4^r - \frac{3}{64\pi^2} \left(\log \frac{M_K^2}{\mu^2} + 1 \right) + \frac{1}{288\pi^2} \frac{M_\pi^2}{M_\eta^2} \right]. \quad (10)$$

The octet radius therefore depends solely on L_5^r , while the other two radii depend on both L_5^r and L_4^r . An accurate determination of the scalar form factors therefore can enable a precise determination of the LECs $\bar{\ell}_4$, and L_5^r and L_4^r , respectively.

In this paper, we determine the scalar form factors of the pion with high statistics and fully controlled systematics, including the extraction of ground state matrix elements, form factor parametrization, and the physical extrapolations. Our form factor data have far better momentum resolution than previous studies due to the use of moving frames, and our determination of the numerically difficult quark-disconnected contribution over the full range of momenta is more than an order of magnitude more accurate than the most precise earlier one. A companion Letter exists in Ref. [3].

This paper is organized as follows: Sec. II includes general information on the ensembles and the setup used in this study, whereas technical aspects of the n -point function and effective form factor calculation are explained in detail in Sec. III. The extraction of ground state matrix elements and the parametrization of the form factors to compute radii are discussed in Secs. IV and V, respectively. The physical extrapolation of our results using χ PT fit ansätze and the determination of LECs is detailed in Sec. VI. Our final results including a full error budget are obtained from model averages in Sec. VII. Finally, Sec. VIII contains a summary and discussion of our findings.

II. ENSEMBLES

The lattice calculation of the form factor in Eq. (2) has been carried out on a set of 17 gauge ensembles listed in Table I that are provided by the Coordinated Lattice Simulations (CLS) consortium [4]. These ensembles feature $N_f = 2 + 1$ flavors of nonperturbatively $O(a)$ -improved Wilson fermions [5] and have been generated with the tree-level Symanzik-improved gauge action [6]. The majority of ensembles exhibit open boundary conditions in the time direction to mitigate the issue of topological freezing [7,8], whereas the remaining ensembles feature periodic boundary conditions. In order to suppress exceptional configurations, a twisted-mass regulator [8] has been introduced in the simulation of the light-quark sector, and the rational approximation has been used for the strange quark [9]. Therefore, the computation of physical observables requires reweighting, and the corresponding reweighting factors have been determined using exact low-mode deflation as described in Ref. [10] for all but one of the ensembles in Table I. The only exception is E300, for which reweighting factors are only available from the conventional stochastic method originally introduced in Ref. [4]. Moreover, we adopt the procedure introduced in Ref. [11] to treat violations of the positivity of the fermion determinant. Such violations have been found to affect a small subset of gauge configurations on some ensembles and can be accounted for in the reweighting procedure by adding a sign to the reweighting factor for a given gauge configuration. In the following, it is implied that the appropriate reweighting has been applied in any gauge average.

The majority of ensembles in Table I lies on the same chiral trajectory defined by a constraint on the trace of the quark mass matrix, i.e., $\text{tr}[M] = 2m_l + m_s = \text{const}$, hence denoted by “ $\text{tr}[M]$.” Additional ensembles have been included that belong to a second chiral trajectory defined by a constant value of the strange quark mass $m_s \approx \text{phys}$ denoted by “ m_s ” in Table I. Since the difference between $F_S^{\pi,0}(Q^2)$ and $F_S^{\pi,8}(Q^2)$ is entirely mediated by the strange quark contribution, we expect this to improve the handle on the combined light and strange quark mass dependence in

TABLE I. List of gauge ensembles used in this study. Superscripts “*o*” and “*p*” denote ensembles with open and periodic boundary conditions in time, respectively. The ensembles fall onto two different chiral trajectories labeled by $\text{tr}[M]$ and m_s that are defined in the text. Values for M_π and M_K have been computed on the same set of configurations, and their errors are dominated by the uncertainty of the scale $\sqrt{t_0}$ in Eq. (11) that is used to convert to physical units. The last three columns list the number of gauge configurations N_{cfg} that have been analyzed, the total number of measurements for quark-connected three-point functions $N_{\text{meas}}^{\text{3pt}}$, and the available number of two-point function measurements $N_{\text{meas}}^{(2+1)\text{pt}}$ used in the computation of the quark-disconnected contributions to the three-point functions.

ID ^{BC}	β	a/fm	$\frac{T}{a} \times (\frac{L}{a})^3$	Traj	L/fm	$M_\pi L$	M_π/MeV	M_K/MeV	N_{cfg}	$N_{\text{meas}}^{\text{3pt}}$	$N_{\text{meas}}^{(2+1)\text{pt}}$
C101 ^o	3.40	0.0855	96×48^3	$\text{tr}[M]$	4.11	4.68	225(2)	476(3)	1970	15760	866800
C102 ^o			96×48^3	m_s	4.11	4.75	228(2)	503(3)	1467	11736	645480
N101 ^o			128×48^3	$\text{tr}[M]$	4.11	5.89	283(2)	466(3)	1577	12616	883120
H102 ^o			96×32^3	$\text{tr}[M]$	2.74	4.97	358(2)	443(3)	2029	16232	1136240
D450 ^p	3.46	0.0756	128×64^3	$\text{tr}[M]$	4.84	5.36	219(1)	480(3)	1009	8072	516608
D451 ^p			128×64^3	m_s	4.84	5.35	218(2)	505(3)	1482	11856	758784
N451 ^p			128×48^3	$\text{tr}[M]$	3.63	5.32	289(2)	465(3)	1004	8032	514048
N452 ^p			128×48^3	$\text{tr}[M]$	3.63	6.50	354(2)	444(3)	998	7984	510976
S400 ^o			128×32^3	$\text{tr}[M]$	2.42	4.37	356(2)	447(3)	993	7944	460752
E250 ^p	3.55	0.0636	192×96^3	both	6.11	4.07	132(1)	494(3)	982	7856	502784
D200 ^o			128×64^3	$\text{tr}[M]$	4.07	4.22	204(1)	485(3)	1984	15872	1111040
D201 ^o			128×64^3	m_s	4.07	4.21	204(1)	505(3)	1062	8496	594720
N200 ^o			128×48^3	$\text{tr}[M]$	3.06	4.45	287(2)	467(3)	1703	13624	953680
N203 ^o			128×48^3	$\text{tr}[M]$	3.06	5.40	349(2)	446(3)	1535	12280	859600
E300 ^o	3.70	0.0493	192×96^3	$\text{tr}[M]$	4.74	4.22	176(1)	495(3)	1134	9072	521640
J303 ^o			192×64^3	$\text{tr}[M]$	3.16	4.17	260(2)	479(3)	1068	8544	598080
J304 ^o			192×64^3	m_s	3.16	4.18	261(2)	526(3)	1625	13000	910000

chiral extrapolations. The two trajectories (approximately) coincide at the physical point; hence, the E250 ensemble is considered part of both trajectories.

Throughout the analysis, dimensionful quantities are expressed in units of the gradient flow scale t_0 [12] using the values for t_0^{sym}/a^2 at the symmetrical point as published in Table III of Ref. [13]. The physical value of t_0 enters the analysis only in the definition of the physical point in the light and strange quark mass and in the conversion of final results to physical units. For the purpose of setting the scale, we use the FLAG world average estimate for $N_f = 2 + 1$ dynamical quark flavors [14]

$$\sqrt{t_0^{\text{phys}}} = 0.14464(87) \text{ fm}. \quad (11)$$

Note that the values for the lattice spacings a in Table I have been computed using the values for $\sqrt{t_0^{\text{phys}}}$ and t_0^{sym}/a^2 . They have only been used for the purpose of converting M_π and M_K in Table I to physical units and do not explicitly enter the actual analysis.

III. COMPUTATIONAL SETUP

Evaluating the matrix elements in Eq. (2) in lattice QCD requires the calculation of two- and three-point functions

$$C_{PP}^{\text{2pt}}(\mathbf{p}, \mathbf{x}_i, t_f - t_i) = \sum_{\mathbf{x}_f} e^{i\mathbf{p} \cdot (\mathbf{x}_f - \mathbf{x}_i)} \langle P(\mathbf{x}_f - \mathbf{x}_i, t_f - t_i) P^\dagger(\mathbf{0}, 0) \rangle_F, \quad (12)$$

$$C_{PS'P}^{\text{3pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{x}_i, t_f - t_i, t_{\text{op}} - t_i) = \sum_{\mathbf{x}_f, \mathbf{x}_{\text{op}}} e^{i\mathbf{p}_f \cdot (\mathbf{x}_f - \mathbf{x}_i)} e^{i\mathbf{q} \cdot (\mathbf{x}_{\text{op}} - \mathbf{x}_i)} \langle P(\mathbf{x}_f - \mathbf{x}_i, t_f - t_i) \mathcal{S}^f(\mathbf{x}_{\text{op}} - \mathbf{x}_i, t_{\text{op}} - t_i) P^\dagger(\mathbf{0}, 0) \rangle_F, \quad (13)$$

where $P(\mathbf{x}, t) = \frac{1}{\sqrt{2}} [\bar{u} \gamma_5 u + \bar{d} \gamma_5 d](\mathbf{x}, t)$ is the usual pseudoscalar interpolating field for the pion, and $\langle \cdot \rangle_F$ denotes fermionic expectation values. Coordinates of initial and

final states are labeled by indices “*i*” and “*f*,” respectively, and the location of the operator insertion is indicated by “op.” In the above expressions, a shift by the source

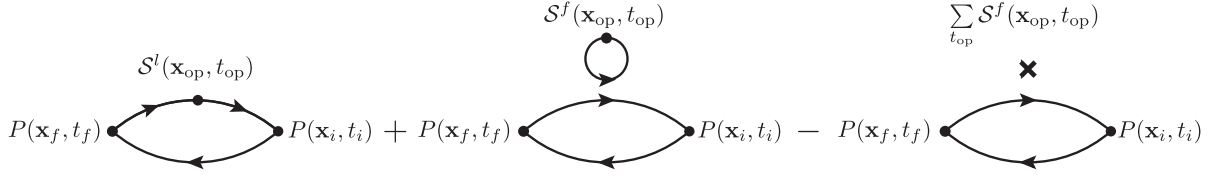


FIG. 1. Quark-connected and disconnected diagrams contributing to the three-point function in Eq. (13). The quark-connected diagram receives only light-quark contributions, while the quark-disconnected contribution depends on the choice of the flavor structure for the operator insertion in Eqs. (4)–(3). The last diagram accounts for the subtraction of the vacuum expectation value that occurs only at vanishing momentum transfer.

position x_i has already been carried out assuming translational invariance.

The Wick contractions for the three-point function in Eq. (13) give rise to quark-connected and quark-disconnected contributions that are diagrammatically depicted in Fig. 1. In the presence of pion initial and final states, the quark-connected diagram contributes only for operator insertions involving light quarks. The quark-disconnected piece, on the other hand, contributes for any quark flavor. Moreover, the scalar current insertion in Eqs. (5)–(3) has vacuum quantum numbers; hence, there is an additional contribution at zero momentum transfer due to a vacuum expectation value (vev) that requires subtraction to obtain physical results, which will be discussed in more detail in Sec. III C.

A. Quark-connected contribution

The quark-connected piece of the three-point function in Fig. 1 is computed to high statistical precision using only a few point sources per gauge field. We employ sequential inversion through the sink [15] and the truncated solver method (TSM) [16–18]. The computations are carried out for a fixed set of source-sink separations $t_{\text{sep}} = t_f - t_i$ (assuming $t_f > t_i$) in lattice units at each value of β as listed in Table II. They are chosen such that always they cover a similar range of physical values, i.e., $t_{\text{sep}} \in [t_{\text{sep}}^{\text{lo}}, t_{\text{sep}}^{\text{hi}}]$ with $t_{\text{sep}}^{\text{lo}} \lesssim 1$ fm and $t_{\text{sep}}^{\text{hi}} \gtrsim 3$ fm. The final state is either produced at rest or with one unit of momentum, i.e., $\mathbf{p}_f = (+1, 0, 0) \cdot 2\pi/L$, which greatly improves the momentum resolution. Since the injection of momenta at the sink requires additional sequential inversions for every single value of $\mathbf{p}_f$, we restrict ourselves to a single

nonvanishing momentum in case of the quark-connected three-point function.

The source setup on individual ensembles depends on the choice of boundary conditions in time: For periodic boundary conditions (pBC), the quark-connected diagrams are evaluated on $N_s^c = 8$ point sources that are randomly selected on every gauge field. The point-to-all propagators are reused for each value of t_{sep} and in the computation of two-point functions. For ensembles with open boundary conditions (oBC), the source setup is chosen symmetric in t around the center of the lattice with two opposing source time slices $t_i = (T - 1 \pm t_{\text{sep}})/2$ at each given value of t_{sep} . This choice restricts the possible source-sink separations to odd values of t_{sep}/a , which is reflected by the values in Table II. We use four point sources on both time slices, averaging over forward and backward diagrams in insertion time $t_{\text{ins}} = t_{\text{op}} - t_i$, such that the number of sources per configuration and source-sink separation remains the same as for pBC ensembles, i.e., $N_s^c = 8$. However, the number of point-to-all propagators now scales with the number of source-sink separations. Again, these are reused for the computation of two-point functions. The total numbers of measurements $N_{\text{meas}}^{\text{3pt}}$ for the quark-connected piece of the three-point function on every ensemble are listed in Table I.

The low-precision solves for two- and three-point functions are averaged over source positions x_i . For ensembles with pBC, this can be done without any restrictions regarding the source time t_i , and we correct for the associated bias on every gauge field using a single high-precision solve on a randomly chosen source position x_i^b , $b \in \{1, \dots, N_s^c\}$; i.e.,

$$C_{PP}^{\text{2pt}}(\mathbf{p}, t) = C_{PP}^{\text{2pt,HP}}(\mathbf{p}, \mathbf{x}_i^b, t_f^b - t_i^b) - C_{PP}^{\text{2pt,LP}}(\mathbf{p}, \mathbf{x}_i^b, t_f^b - t_i^b) + \frac{1}{N_s^c} \sum_{j=1}^{N_s^c} C_{PP}^{\text{2pt,LP}}(\mathbf{p}, \mathbf{x}_i^j, t_f^j - t_i^j), \quad (14)$$

$$\begin{aligned} C_{PS'P}^{\text{3pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}}) &= C_{PS'P}^{\text{3pt,HP}}(\mathbf{p}_f, \mathbf{q}, \mathbf{x}_i, t_f^b - t_i^b, t_{\text{op}}^b - t_i^b) - C_{PS'P}^{\text{3pt,LP}}(\mathbf{p}_f, \mathbf{q}, \mathbf{x}_i, t_f^b - t_i^b, t_{\text{op}}^b - t_i^b) \\ &+ \frac{1}{N_s^c} \sum_{j=1}^{N_s^c} C_{PS'P}^{\text{3pt,LP}}(\mathbf{p}_f, \mathbf{q}, \mathbf{x}_i, t_f^j - t_i^j, t_{\text{op}}^j - t_i^j), \end{aligned} \quad (15)$$

TABLE II. Lower and upper bounds $t_{\text{sep}}^{\text{lo}}$ and $t_{\text{sep}}^{\text{hi}}$ as well as the stride between to consecutive values of t_{sep} for which three-point function data has been computed.

β	$t_{\text{sep}}^{\text{lo}}/a$	$t_{\text{sep}}^{\text{hi}}/a$	$\Delta t_{\text{sep}}/a$
3.40	11	35	4
3.46	13	41	4
3.55	15	51	6
3.70	19	67	8

where we have introduced the usual time indexing $t = t_f^j - t_i^j$ for the two-point function and made the $\mathbf{p}_i$ dependence of the three-point function explicit in its argument list. Superscripts “HP” and “LP” refer to high- and low-precision solves, respectively. On the other hand, for ensembles with oBC, the source average is performed at any given value of t_{sep} , averaging only over the forward and backward contributions in t_{ins} obtained from the two contributing source time slices with $t_i = (T - 1 \pm t_{\text{sep}})/2$. The bias correction is carried out on a randomly selected (spatial) source for each of the two values of t_i on every individual gauge configuration.

For the extraction of effective form factors, we average over equivalent momenta before forming ratios. To this end, we define equivalence classes $\mathbf{p} = \{\tilde{\mathbf{p}} \in \mathbb{P}^3 | \tilde{\mathbf{p}}^2 = \mathbf{p}^2\}$, where $\mathbb{P}^3 = \{\mathbf{p} = \frac{2\pi}{L} \mathbf{n} | \mathbf{n} \in \mathbb{Z}^3\}$ denotes the set of lattice three-momenta. Carrying out the corresponding momentum average for the two-point function in Eq. (12) yields

$$C_{PP}^{2\text{pt}}(\mathbf{p}, t) = \frac{1}{N_{\mathbf{p}}} \sum_{\mathbf{p} \in \mathbf{p}} C_{PP}^{2\text{pt}}(\mathbf{p}, t), \quad (16)$$

where $N_{\mathbf{p}}$ denotes the number of distinct lattice momenta $\mathbf{p}$ in the class $\mathbf{p}$, and we have defined $t = t_f - t_i$. Similarly, for three-point functions, we introduce classes of momentum triplets $(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i) = \{(\tilde{\mathbf{p}}_f, \tilde{\mathbf{q}}, \tilde{\mathbf{p}}_i) \in \mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3 | (\tilde{\mathbf{p}}_f^2, \tilde{\mathbf{q}}^2, \tilde{\mathbf{p}}_i^2) = (\mathbf{p}_f^2, \mathbf{q}^2, \mathbf{p}_i^2)\}$. Since they are unambiguously defined by triplets of squared lattice momenta, it is convenient to introduce corresponding labels $\mathcal{P} = \{n(\mathbf{p}_f^2), n(\mathbf{q}^2), n(\mathbf{p}_i^2)\}$ with $n(\mathbf{p}^2) = \mathbf{p}^2 \cdot (L/2\pi)^2$. Again, we average the three-point functions over equivalent momenta and source positions x_i

$$C_{PS'P}^{3\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}}) = \frac{1}{N_{\mathcal{P}}} \sum_{(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i) \in (\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i)} C_{PS'P}^{3\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}}), \quad (17)$$

where $N_{\mathcal{P}}$ denotes the multiplicity of momenta in any given class $(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i)$.

The computation of the effective form factor requires the cancellation of unknown overlap factors, which can be achieved in the standard way by forming a ratio of two- and three-point functions

$$R^f(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}}) = \frac{\langle C_{PS'P}^{3\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}}) \rangle}{\langle C_{PP}^{2\text{pt}}(\mathbf{p}_f, t_{\text{sep}}) \rangle} \sqrt{\frac{\langle C_{PP}^{2\text{pt}}(\mathbf{p}_i, t_{\text{sep}} - t_{\text{ins}}) \rangle \langle C_{PP}^{2\text{pt}}(\mathbf{p}_f^2, t_{\text{ins}}) \rangle \langle C_{PP}^{2\text{pt}}(\mathbf{p}_f^2, t_{\text{sep}}) \rangle}{\langle C_{PP}^{2\text{pt}}(\mathbf{p}_f^2, t_{\text{sep}} - t_{\text{ins}}) \rangle \langle C_{PP}^{2\text{pt}}(\mathbf{p}_i^2, t_{\text{ins}}) \rangle \langle C_{PP}^{2\text{pt}}(\mathbf{p}_i^2, t_{\text{sep}}) \rangle}}, \quad (18)$$

where $\langle \cdot \rangle$ indicates gauge averages. Note that for a scalar operator insertion, the form factor decomposition is trivial; i.e., $R^f(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}})$ up to excited state contamination directly yields the unrenormalized matrix elements without additional kinematic structures. For the quark-connected contribution to $C_{PS'P}^{3\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}})$, a favorable signal-to-noise behavior for $R^f(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}})$ is obtained by evaluating two- and three-point functions on the exact same set of sources, as opposed to using full available statistics for the two-point functions. In particular, for ensembles with oBC, we neither average over source positions t_i contributing to different values of t_{sep} in the quark-connected part of $C_{PS'P}^{3\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}})$ nor do we include additional two-point function measurements required for the computation of $(2+1)$ -point quark-disconnected diagrams that will be discussed below. To further optimize

correlations for the evaluation of Eq. (18), the two-point functions are not averaged over forward and backward time direction, but we rather choose the time direction that coincides with the t_{ins} indexing of $C_{PS'P}^{3\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}})$, i.e., forward direction on ensembles with pBC and forward (backward) direction on ensembles with oBC for $t_i < T/2$ ($t_i > T/2$), as explained before.

Statistical errors for any observable are always computed and propagated using the nonparametric bootstrap method with $N_B = 1000$ bootstrap samples and binning to account for autocorrelation. Similar to what has been observed previously for isoscalar nucleon structure observables in Refs. [19–21], a few measurement on individual point sources show up as extreme outliers in the corresponding distribution across gauge configurations. While this affects only very small subset of gauge fields, these measurements would spoil the expected scaling behavior of the statistical

error with the total number of measurements as well as the expected signal-to-noise ratio as a function of t_{sep} , t_{ins} . Moreover, including them causes a generally unreasonable increase of statistical errors. Therefore, we have implemented a similar procedure as the one discussed in the supplemental material of Ref. [19] to flag these measurements and remove them from the computation of gauge averages. For this purpose, we generate single-elimination jackknife samples for the effective form factors on the full set of data and scan them for results that are further away than $\sim 6\sigma$ from the center of the sample distribution. Any gauge configurations identified by this procedure is then removed from the actual (bootstrap-based) analysis. This elimination is already reflected by the number of gauge configurations N_{conf} listed in Table I.

B. Quark-disconnected contribution

The numerical evaluation of the quark-disconnected contribution to Eq. (13) requires the computation of two-point functions $C_{PP}^{2\text{pt}}(\mathbf{p}_f, \mathbf{x}_i, t)$ and scalar quark loops

$$L_{Sf}(\mathbf{q}, t) = -\sum_{\mathbf{x}} e^{i\mathbf{q}\cdot\mathbf{x}} \text{tr}[D_f^{-1}(x, x)], \quad (19)$$

where $D_f^{-1}(x, x)$ denotes the self-contracted all-to-all propagator for a quark flavor $f = l, s$. The computation of these loops has been carried out on all ensembles in the scheme that we have introduced in Ref. [22] based on the

method in Ref. [23], combining the one-end trick (OET) [24], the generalized hopping parameter expansion (gHPE) [25], and hierarchical probing (HP) [26]. In this scheme, quark loops are computed for any local bilinear or one-link displaced operator without incurring additional inversion cost for individual operators, facilitating their (re)use in various other projects; e.g., in nucleon structure calculations in Refs. [19–21], as well as the hadronic vacuum polarization and hadronic light-by-light contributions to $g - 2$ in Refs. [27–29].

The measurements for the pion two-point function that are obtained from the forward propagators of the quark-connected three-point functions are generally insufficient to achieve a statistically precise signal for the quark-disconnected contribution in Fig. 1. Therefore, we have carried out a dedicated effort to increase statistics for the two-point functions. Again, the numerical setup for these additional measurements as well as evaluation of the $(2+1)$ -point contributions depends on the choice of the boundary conditions in time. For pBC ensembles, additional source positions can be randomly distributed on each configuration such that the number of measurement per gauge configuration is increased to $N_s^d = 512$ on every ensemble. Unlike for the quark-connected piece, forward and backward averaging in t_{ins} does not incur additional cost for inversions. Therefore, we increase statistics for any source position x_i of the two-point function by averaging over the two contributions

$$C_{PSfP}^{(2+1)\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, \mathbf{x}_i, t_{\text{sep}}, t_{\text{ins}}) = C_{PP}^{2\text{pt}}(\mathbf{p}_f, \mathbf{x}_i, t_{\text{sep}}) \tilde{L}_{Sf}(\mathbf{q}, t_{\text{ins}}) e^{-i\mathbf{q}\mathbf{x}_i}, \quad (20)$$

$$C_{PSfP}^{(2+1)\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, \mathbf{x}_i, T - t_{\text{sep}}, T - t_{\text{ins}}) = C_{PP}^{2\text{pt}}(\mathbf{p}_f, \mathbf{x}_i, T - t_{\text{sep}}) \tilde{L}_{Sf}(\mathbf{q}, T - t_{\text{ins}}) e^{-i\mathbf{q}\mathbf{x}_i}, \quad (21)$$

where the indexing of the loop has been assumed to be implicitly shifted by t_i , i.e., $\tilde{L}_{Sf}(\mathbf{q}, t) = L_{Sf}(\mathbf{q}, t + t_i)$. The implementation of the TSM for the two-point function in Eq. (14) is straightforwardly extended to the $(2+1)$ -point case. Since the final state momentum $\mathbf{p}_f$ in Eqs. (20) and (21) is determined by the two-point function contribution, all signed permutations contributing to one unit of final state momentum can be computed without additional inversions, increasing the statistical precision for the resulting signal. The computation of the ratio in Eq. (18) for any flavor structure f then proceeds in the same way as for the quark-connected piece by computing gauge averages and averaging two- and three-point functions over equivalent momenta as discussed in Sec. III A. In order to optimize correlations in $R^f(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}})$, we evaluate the $(2+1)$ -point and two-point functions on exactly the same (extended) set of 512 source positions. Moreover, we average also the two-point functions in the ratio themselves over forward and backward contributions in t .

For ensembles with oBC, the evaluation of the quark-disconnected diagrams and the placement of additional sources for two-point functions become more intricate as boundary effects must be avoided in the construction of n -point functions. First of all, they result in excited state contamination in, e.g., the scalar one-point function at zero-momentum $L_{Sf}(\mathbf{0}, t)$ as shown in Fig. 2 for the E300 ensemble. The regions where the signal for the vev $L_{Sf}(\mathbf{0}, t)$ exhibits a nonconstant t dependence must be excluded for the computation of the quark-disconnected diagrams; i.e., we restrict $L_{Sf}(\mathbf{p}, t)$ to $t_i \in [t_{\text{ex}}, T - t_{\text{ex}}]$. The values of t_{ex} generally depend on M_π and have been listed in Table III. Similarly, we restrict the time slices for two-point function sources to $t_i \in [t_{\text{ex}}, T - t_{\text{ex}}]$. Statistics for the two point function are increased by incrementally adding pairs of time slices starting at t_{ex} and $T - t_{\text{ex}}$ toward the center of the lattice until the target statistics of $N_s^d \geq 512$ per configuration is reached or no more time slices are available; cf. Table III. For ensembles at $\beta = 3.7$

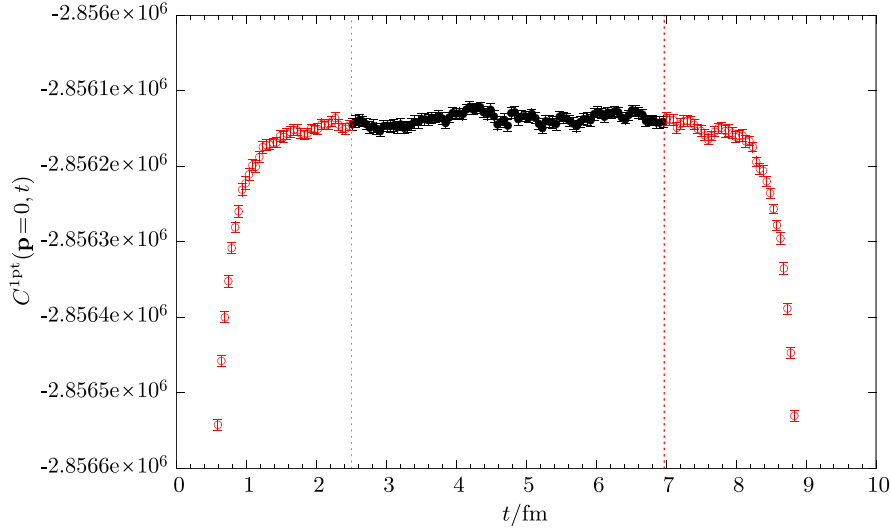


FIG. 2. Time dependence of the scalar one-point function with nonvanishing vacuum expectation value on the E300 ensemble with open boundary conditions. The vertical dashed lines mark the exclusion zone next to the boundaries (see text), and the red data are discarded in the computation of quark-disconnected $(2+1)$ -point functions to avoid excited-state contamination due to boundary effects.

(and S400), we use only every second time slice in this procedure, whereas for all other ensembles, every value of t_i is allowed. Again, the bias correction for the TSM has been performed on a single, randomly selected (spatial) source every value of t_i . Besides, we carry out additional measurements on the time slices used in the computation of the quark-connected contribution such that the number of two-point function measurements per time slice is the same for every value of t_i .

For the evaluation of Eqs. (20) and (21), not only the source time slice t_i of $C_{PP}^{2pt}(\mathbf{p}_f, \mathbf{x}_i, t_f - t_i)$ but also t_f must remain within $[t_{\text{ex}}, T - t_{\text{ex}}]$. This implies an additional, severe constraint on the effective statistics as t_i is restricted to two strips, i.e., $t_i \in [t_{\text{ex}}, T - t_{\text{ex}} - t_{\text{sep}}]$ and $t_i \in [t_{\text{ex}} + t_{\text{sep}}, T - t_{\text{ex}}]$, which linearly shrink for increasing

values of t_{sep} . Therefore, the values of N_s^d as listed in Table III are merely an upper bound on the actual statistics. Anyhow, we still average over forward and backward contributions in t_{ins} whenever the choice of t_{sep} and t_i allows for it, but the gain of statistics from this is very limited compared to the case of pBC in time.

C. Vacuum expectation value subtraction at $\mathbf{q} = \mathbf{0}$

At vanishing momentum transfer, the scalar quark loops feature a nonvanishing vev $\langle L_{S^f}(\mathbf{q} = \mathbf{0}, t) \rangle \neq 0$ that requires subtraction to obtain physical results. Assuming pBC in time, this can be achieved in the standard way, i.e., by subtracting

$$\langle C_{PS^fP}^{\text{vev}}(\mathbf{p}_f, \mathbf{q} = \mathbf{0}, t_{\text{sep}}) \rangle_{\text{pBC}} = \langle C_{PP}^{2pt}(\mathbf{p}_f, t_{\text{sep}}) \rangle \cdot \frac{1}{T} \sum_{t=0}^{T-1} \langle L_{S^f}(\mathbf{0}, t) \rangle, \quad (22)$$

from the rhs of Eqs. (20) and (21) for $\mathbf{q} = \mathbf{0}$, $\mathbf{p}_f = \mathbf{p}_i$ after taking the appropriate source and gauge averages. In principle, a similar expression could be used for oBC in time

$$\langle C_{PS^fP}^{\text{vev}}(\mathbf{p}_f, \mathbf{q} = \mathbf{0}, t_{\text{sep}}) \rangle_{\text{oBC}} = \langle C_{PP}^{2pt}(\mathbf{p}_f, t_{\text{sep}}) \rangle \cdot \frac{1}{T - 2t_{\text{ex}}} \sum_{t=t_{\text{ex}}}^{T-t_{\text{ex}}-1} \langle L_{S^f}(\mathbf{0}, t) \rangle, \quad (23)$$

excluding the regions affected by boundary effects in the t average of the loop. However, we observe that this naive ansatz leads to unacceptably large fluctuations in the effective form factor signal on several ensembles. An example for this is shown in Fig. 3 for the flavor singlet

and octet quark-disconnected contributions to the effective form factor on the C101 ensemble. This effect is caused by insufficient sampling of the quark loop in the evaluation of the quark-disconnected contribution due to the aforementioned restrictions on the placement of point sources for the

TABLE III. Values of t_{ex} defining the exclusion regions next to the boundaries in time for ensembles and the number of available two-point function measurements for the construction of $(2+1)$ -point quark-disconnected diagrams N_s^d on these ensembles.

ID	t_{ex}/a	N_s^d
C101	26	440
C102	26	440
N101	23	548
H102	20	548
S400	23	464
D200	35	548
D201	35	548
N200	31	548
N203	27	548
E300	50	448
J303	40	548
J304	40	548

two-point functions. As a result, local fluctuations in the signal of the loop in t are not adequately averaged out. On the other hand, subtracting the “naive” estimator for the vev in Eq. (23) does not compensate such fluctuations but only

amounts to a constant shift of the signal for the resulting three-point function. Since the vev of the loop is several orders of magnitude larger than the signal of the final three-point function, these fluctuations may easily dominate the signal, hindering further analysis. The issue becomes increasingly more severe at larger values of t_{sep} as the available source time slices are further reduced. For example, at the largest value of $t_{\text{sep}} = 35a$ on the C101 ensemble, the size of the two strips next to the regions excluded for source placement in t shrink to $\lesssim 0.4$ fm amounting to only a handful of time slices for the two-point functions.

A remedy for these fluctuations is found by implementing a modified estimator for the effective form factor at $\mathbf{q}^2 = 0$. Instead of computing global gauge averages of Eqs. (20) and (21) including any source position x_i , we restrict them to individual source time slices t_i . The corresponding expressions $\langle C_{PS'P}^{(2+1)\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_i, t_{\text{sep}}, t_{\text{ins}}) \rangle$ and $\langle C_{PS'P}^{(2+1)\text{pt}}(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_i, T - t_{\text{sep}}, T - t_{\text{ins}}) \rangle$ are averaged only over spatial source positions $\mathbf{x}_i$ on the same source time slice t_i . Consequently, we introduce a modified estimator for the vev subtraction

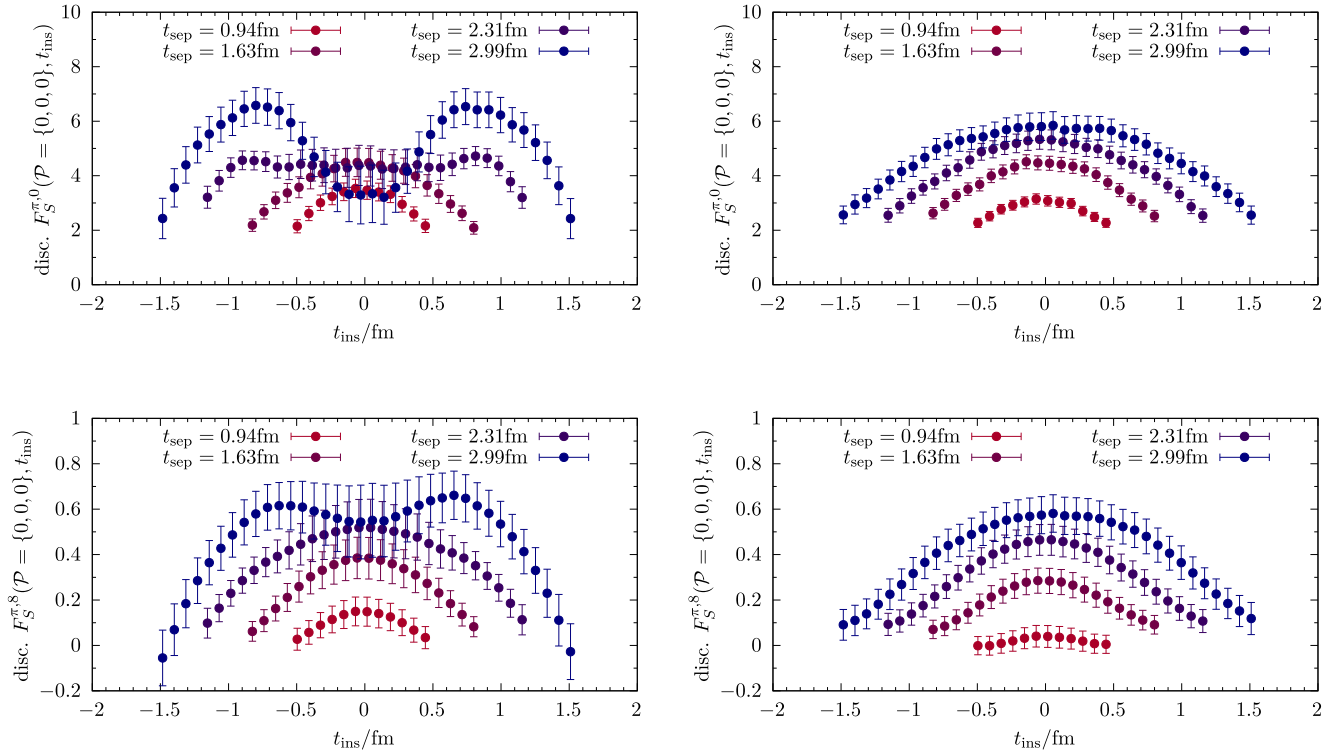


FIG. 3. Comparison of the quark-disconnected contribution to the (unrenormalized) effective form factor at vanishing momentum transfer using the two different methods for the subtraction of the vacuum expectation value on the C101 ensemble with open boundary conditions. Left column: “naive” subtraction as defined in Eq. (23); right column: improved, time-slice-wise method as defined in Eq. (24). Results are shown for the flavor singlet (top row) and octet (bottom row) combinations. Data at every second available value of t_{sep} have been included and displaced horizontally for better legibility.

$$\begin{aligned} & \langle C_{PS^fP}^{\text{vev}}(\mathbf{q} = \mathbf{0}, t_i, t_{\text{sep}}, t_{\text{ins}}) \rangle_{\text{oBC}} \\ &= \langle C_{PP}^{2\text{pt}}(\mathbf{p}_f, t_i, t_{\text{sep}}) \rangle \langle \tilde{L}_{S^f}(\mathbf{0}, t_{\text{ins}}) \rangle; \end{aligned} \quad (24)$$

i.e., we perform the subtraction for every value of t_i separately and without an average in the operator insertion

$$R_{\text{disc}}^f(\mathbf{p}_f, \mathbf{q} = \mathbf{0}, \mathbf{p}_i = \mathbf{p}_f, t_{\text{sep}}, t_{\text{ins}}) = \frac{1}{N_{t_i}(t_{\text{sep}})} \sum_{t_i} \frac{\langle C_{PS^fP}^{3\text{pt}}(\mathbf{p}_f, \mathbf{q} = \mathbf{0}, \mathbf{p}_i = \mathbf{p}_f, t_i, t_{\text{sep}}, t_{\text{ins}}) \rangle_{\text{disc}}}{\langle C_{PP}^{2\text{pt}}(\mathbf{p}_f, t_i, t_{\text{sep}}) \rangle}, \quad (25)$$

where $N_{t_i}(t_{\text{sep}})$ denotes the number of contributing source time slices at any given value of t_{sep} , and gauge averages of the two-point function $\langle C_{PP}^{2\text{pt}}(\mathbf{p}_f, t_i, t_{\text{sep}}) \rangle$ have been computed per time slice as well. As can be seen comparing the right panels of Fig. 3 to the ones on the left, this procedure entirely removes the fluctuations that otherwise distort the signal for the quark-disconnected contribution to the form factor. Moreover, it leads to a significant reduction of the point error by a factor up to 2, exploiting statistical correlations time slice by time slice.

IV. EXTRACTION OF GROUND STATE MATRIX ELEMENTS

The extraction of ground-state matrix elements for the pion scalar form factor in Eq. (2) from lattice data requires control over excited state contamination. For this purpose, we employ the summation method [30–33]

$$\begin{aligned} \sum_{t_{\text{ins}}=\tau}^{t_{\text{sep}}-\tau} R^f(\mathbf{p}_f, \mathbf{q}, \mathbf{p}_i, t_{\text{sep}}, t_{\text{ins}}) &= \text{const} + \langle \pi(\mathbf{p}_f) | S^f | \pi(\mathbf{p}_i) \rangle \\ &\times (t_{\text{sep}} - \tau) + \mathcal{O}(e^{-\Delta t_{\text{sep}}}), \end{aligned} \quad (26)$$

where Δ denotes the energy gap between ground and first excited state. The matrix element is extracted from a correlated linear fit in $t_{\text{sep}} \in [t_{\text{sep}}^{\min}, t_{\text{sep}}^{\max}]$, where we choose $1.0 \text{ fm} \lesssim t_{\text{sep}}^{\min} \lesssim 1.5 \text{ fm}$ and $2.5 \text{ fm} \lesssim t_{\text{sep}}^{\max} \lesssim 3.0 \text{ fm}$, using three values for $t_{\text{sep}}^{\min}$ and $t_{\text{sep}}^{\max}$ each. The remaining analysis is carried out for all resulting $(t_{\text{sep}}^{\min}, t_{\text{sep}}^{\max})$ pairs to account for systematic effects due to possible residual excited state contamination at smaller values of t_{sep} , as well as potential issues due the decreasing statistical precision of the quark-disconnected piece at large values of t_{sep} in case of ensembles with oBC in time. Furthermore, we always choose $t_{\text{ex}} = t_{\text{sep}}^{\min}/2$, i.e., the most restrictive choice possible, which we find to yield the best statistical precision and most stable fits in the presence of nonvanishing momentum transfer. The reason for this is that increasing $|\mathbf{p}_i|$ (or $|\mathbf{p}_f|$) causes a deterioration of the signal in t_{ins} close to $t_i(t_f)$; hence, excluding as many noisy data points as possible improves the quality of the resulting signal. We

time. This correlated subtraction leads to a cancellation of residual fluctuations in the quark-loop time dependence. The final average over source time slices t_i is only carried out after building the ratio. Specifically, we replace the quark-disconnected contribution to the ratio in Eq. (18) by

remark that at least at vanishing momentum transfer, ground state saturation can also be achieved by the plateau (or midpoint) method for sufficiently large values of $t_{\text{sep}} \gtrsim 2.5 \text{ fm}$, as can be inferred from the effective form factors shown in the left column of Fig. 4. This is because there is no signal-to-noise problem for the pion at rest. Note that the excited state contamination in the full effective form factors including the quark-disconnected contribution is enhanced compared to the quark-connected part; i.e., the latter exhibits ground state saturation already for $t_{\text{sep}} \gtrsim 1.5 \text{ fm}$. Anyhow, the summation method is much less prone to fluctuations in the input data than the plateau method, and it yields compatible but statistically more precise results. In particular, it allows including data at smaller values of t_{sep} because excited states are parametrically more strongly suppressed by $e^{-\Delta t_{\text{sep}}}$ compared to $e^{-\Delta t_{\text{sep}}/2}$ for, e.g., the midpoint method. Finally, we remark that injecting one unit of momentum at the sink of the quark-connected piece generally leads to a statistically much more precise signal than injecting at the source. This behavior is expected as the sequential source averages over the entire time slice, projecting cleanly onto momentum eigenstates and improving overlap. In contrast, point sources have poor overlap with moving states, making momentum injection at the source much noisier.

Besides the summation method, we have also attempted multistate fits to extract the ground state matrix elements, explicitly fitting the time dependence in t_{sep} and t_{ins} simultaneously. However, we find that such fits suffer from severe stability issues due to the large covariance matrices and the very strong correlations in the ratio data.

The emerging signal-to-noise problem at nonvanishing values of $\mathbf{p}_i$ and $\mathbf{p}_f$ affects not only the three-point function but also the two-point functions that enter the ratio in Eq. (18). This becomes an issue at larger values of t_{sep} as $C_{PP}^{2\text{pt}}(\mathbf{p}, t)$ enters the ratio for any value $t \in [0, t_{\text{sep}}]$. An example is shown in Fig. 5 for the E300 ensemble with two-point function statistics corresponding to the quark-connected and disconnected three-point function at $t_{\text{sep}} = 59a$. However, because $C_{PP}^{2\text{pt}}(\mathbf{p}, t)$ reaches ground-state saturation for $t \gtrsim 1.5 \text{ fm}$ on every ensemble, the signal quality for the ratio can be improved by fitting the ground state of the

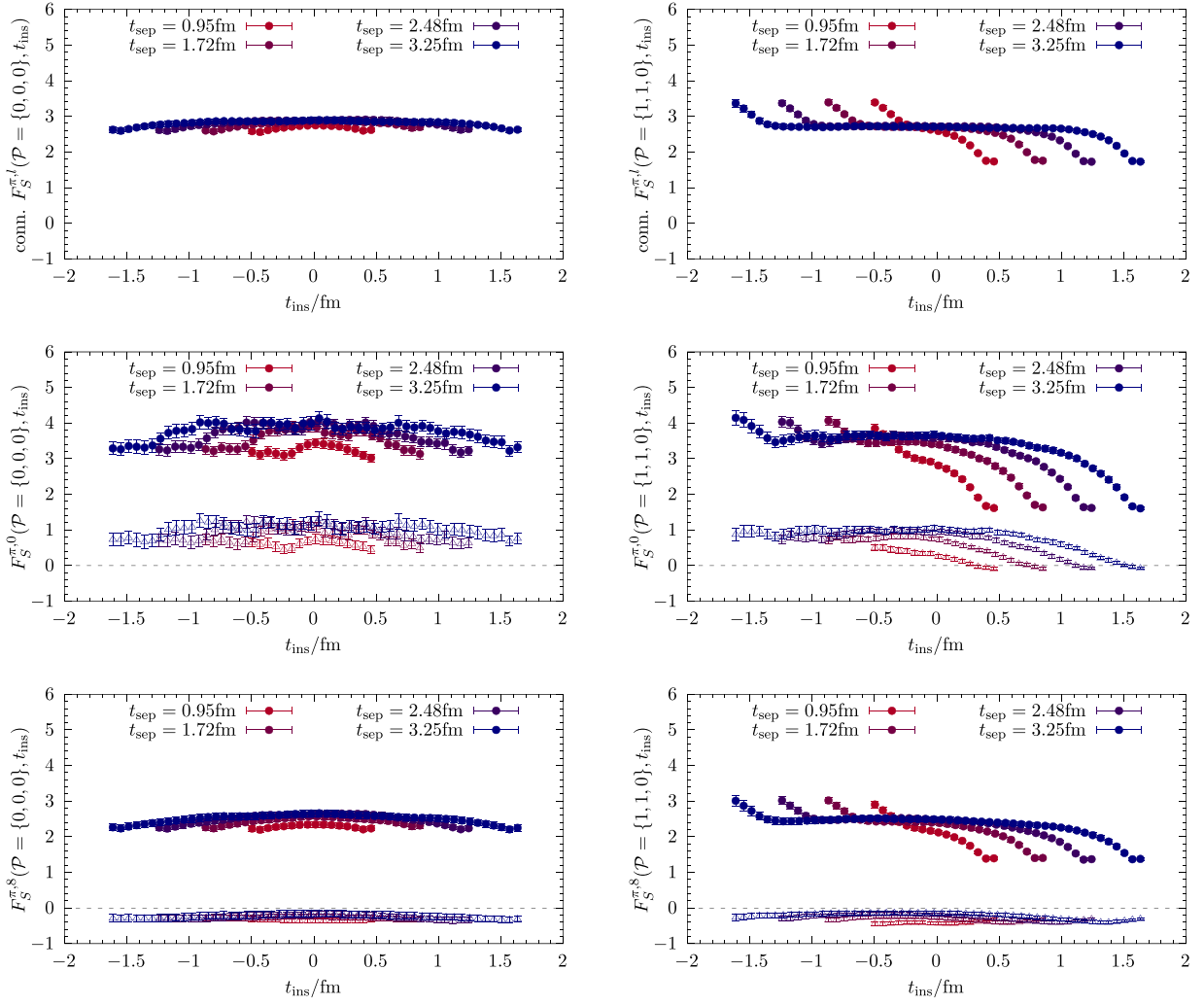


FIG. 4. Effective form factors on the E250 ensemble for every second available value of t_{sep} . Results are shown (from top to bottom) for the quark-connected, the flavor singlet, and octet combinations. For the flavor singlet and octet combinations, the full signal (filled symbols) and the quark-disconnected contribution (open symbols) have been included in the same panel. $\mathcal{P} = \{\mathbf{p}_f^2, \mathbf{q}^2, \mathbf{p}_i^2\}$ indicates the momentum configuration, i.e., vanishing momentum transfer and sink momentum (left column), and one unit of momentum transfer at nonvanishing sink momentum (right column). Data at different values of t_{sep} have been displaced horizontally for better legibility.

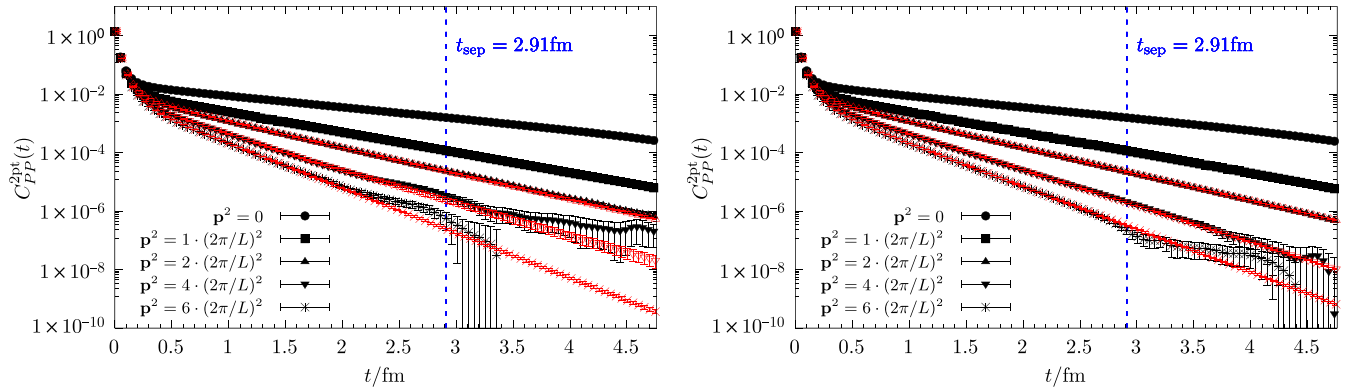


FIG. 5. Signal for the two-point correlation function $C_{PP}^{2pt}(\mathbf{p}, t)$ (black symbols) on the E300 ensemble at several values of $\mathbf{p}^2$. For $\mathbf{p}^2 \geq 2 \cdot (2\pi/L)^2$, the lattice data are replaced by the reconstructed signal (red symbols) that is obtained by replacing the large- t tail with a fit of the ground state contribution. Results are shown for two-point statistics matching the quark-connected three-point function (left panel) and with quark-disconnected (2 + 1)-point function (right panel) at $t_{\text{sep}} = 59a \approx 2.91$ fm.

two-point function and replacing its tail by the fit, which is statistically much more precise than the available lattice data at large values of t . To this end, we fit $C_{PP}^{2pt}(\mathbf{p}, t)$ with a single state for $t \in [t_1, t_2]$, where t_1 is determined by an automatic scan on every ensemble for each value of $\mathbf{p}^2$, and t_2 is chosen to be the last data point for which the signal is not yet lost in noise. The reconstructed signal is then obtained by replacing $C_{PP}^{2pt}(\mathbf{p}, t \geq t_1)$ with the fitted result on every bootstrap sample. While the momentum resolution can be very different depending on the ensemble, we find $\mathbf{p}_{\min}^2 = 2 \cdot (\pi/L)^2$ to be generally a reasonable choice for the smallest momentum from which on to employ this procedure.

V. FORM FACTOR PARAMETRIZATION

The extraction of the scalar radius in Eq. (1) requires a parametrization of the lattice data for $F_S^{\pi,f}(Q^2)$ that is obtained at discrete values of Q^2 . Previous lattice studies relied on rather crude linear interpolations between $F_S^{\pi,f}(0)$ and $F_S^{\pi,f}(Q^2)$ at the first nonvanishing momentum, as the required quark-disconnected contributions to $F_S^{\pi,f}(Q^2)$ could only be computed for one or two nonvanishing values of Q^2 ; see, e.g., Refs. [25,34,35]. Our present set of data allows us to reliably track $F_S^{\pi,f}(Q^2)$ for a much larger range of Q^2 values and with a fine-grained momentum resolution, especially on lattices with large physical volume as shown in Fig. 6. We observe that adding data with one

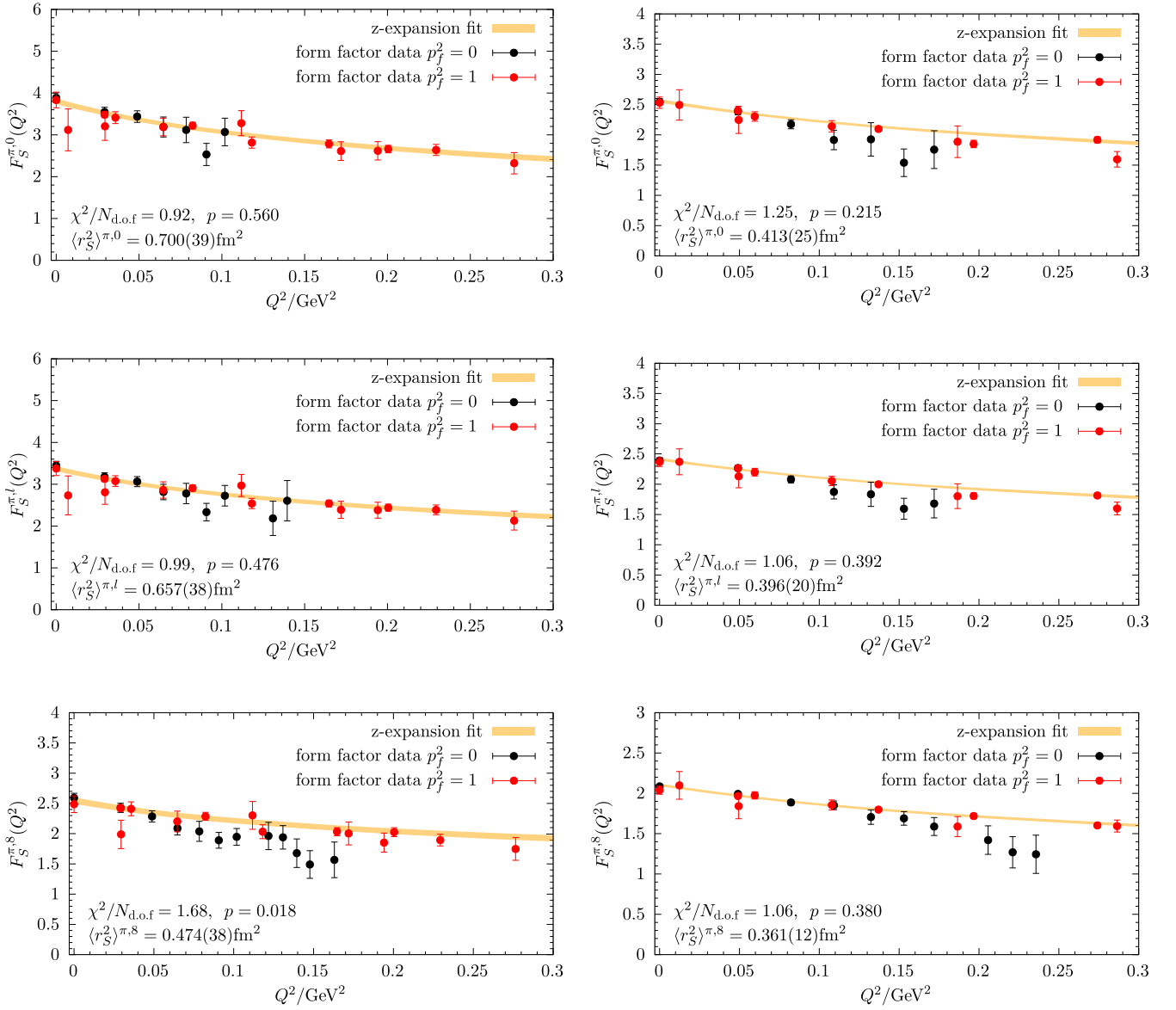


FIG. 6. Form factor data and z-expansion fit bands for $F_S^{\pi,0}(Q^2)$ (top), $F_S^{\pi,l}(Q^2)$ (center), and $F_S^{\pi,8}(Q^2)$ (bottom) on the two most chiral ensembles E250 (left column) and E300 (right panel). Results are shown for the data set including source-sink separations with $1.25 \text{ fm} \leq t_{\text{sep}} \leq 3.25 \text{ fm}$ and a cut in the momentum transfer of $Q^2 \leq 0.3 \text{ GeV}^2$.

unit of sink momentum greatly enhances the accessible range and resolution as well as the overall statistical quality of the signal. Therefore, we make use of a z -expansion fit ansatz [36] to parametrize the Q^2 dependence

$$F_S^{\pi,f}(Q^2) = \sum_{n=0}^{N_z} a_n^f z^n, \quad z = \frac{\sqrt{t_{\text{cut}} + Q^2} - \sqrt{t_{\text{cut}} - t_0}}{\sqrt{t_{\text{cut}} + Q^2} + \sqrt{t_{\text{cut}} - t_0}}, \quad (27)$$

where we use $N_z = 1$, $t_{\text{cut}} = 4M_\pi^2$ and $t_0 = t_0^{\text{opt}} = t_{\text{cut}}(1 - \sqrt{1 + Q_{\text{max}}^2/t_{\text{cut}}})$ [37]. We find that increasing the order of the expansion $N_z \gg 1$ typically only inflates the error on the extracted radii $\langle r_S^2 \rangle_\pi^f \sim a_1^f$ without improving the quality of the fits. In particular, for the most chiral ensembles E250 and E300, these fits yield an excellent description of the lattice data at the present level of statistics; cf. Fig. 6. Anyhow, all fits are carried out for five different maximum values of the momentum transfer $Q_{\text{max}}^2 \in \{0.2, 0.25, 0.3, 0.35, 0.4\}$ GeV to account for residual higher-order effects in the final error budget. We remark that there can be

up to 125 distinct Q^2 values depending on the ensemble. Therefore, we have pruned the data that enter the fits (and Fig. 6) by demanding that the relative point errors do not exceed 20% in case of $F_S^{\pi,0}(Q^2)$, $F_S^{\pi,l}(Q^2)$ and 10% for $F_S^{\pi,8}(Q^2)$, which is inherently more precise. This leaves the fit results virtually unchanged as they are dominated by statistically much more precise data, but it prevents potential issues that may arise from estimating large and noisy covariance matrices in correlated fits.

VI. PHYSICAL EXTRAPOLATIONS

For the physical extrapolations of the scalar radii, we employ fit ansätze that are based on the corresponding NLO SU(3) χ PT expressions. They are obtained by rewriting Eqs. (7)–(10) in terms of leading-order quark mass proxies $\xi_l = t_0 M_\pi^2$ and $\xi_s = t_0(2M_K^2 - M_\pi^2)$, using the leading-order Gell-Mann–Okubo relation $3M_\eta^2 = 4M_K^2 - M_\pi^2$, and expressing all dimensionful observables in units of t_0

$$\frac{\langle r_S^2 \rangle_\pi^0}{t_0} = \frac{1}{(4\pi\sqrt{t_0}f_0)^2} \left[768\pi^2(3L_4^r + L_5^r) - 19 + \frac{\xi_l}{\xi_l + 2\xi_s} - 12\log(\xi_l) - 6\log\left(\frac{\xi_l + \xi_s}{2}\right) \right], \quad (28)$$

$$\frac{\langle r_S^2 \rangle_\pi^l}{t_0} = \frac{1}{(4\pi\sqrt{t_0}f_0)^2} \left[768\pi^2(2L_4^r + L_5^r) - 16 + \frac{\xi_l}{3(\xi_l + 2\xi_s)} - 12\log(\xi_l) - 3\log\left(\frac{\xi_l + \xi_s}{2}\right) \right], \quad (29)$$

$$\frac{\langle r_S^2 \rangle_\pi^8}{t_0} = \frac{1}{(4\pi\sqrt{t_0}f_0)^2} \left[768\pi^2 L_5^r - 10 - \frac{\xi_l}{\xi_l + 2\xi_s} - 12\log(\xi_l) + 3\log\left(\frac{\xi_l + \xi_s}{2}\right) \right]. \quad (30)$$

The scale dependence μ has been absorbed into the definitions of $L_{4,5}^r$, implicitly setting $\sqrt{t_0}\mu = 1$ in the fits. In order to determine the physical values of the radii on any given set of input data, we individually fit the above expressions complemented by a term $\sim a^2/t_0$ with a free fit parameter to account for the continuum extrapolation. The physical point in the light and strange quark mass proxies is defined in the isospin limit using $M_\pi^{\text{phys}} = 134.8(3)$ MeV and $M_K^{\text{phys}} = 494.2(3)$ MeV from Ref. [38].

In addition to fitting the full set of lattice data, we apply a set of data cuts to test for systematic effects in the physical extrapolations. First of all, we have implemented three different cuts in M_π , i.e., $M_\pi < M_\pi^{\text{cut}} \in \{230, 265, 290\}$ MeV, to test for residual higher-order effects in the light quark mass beyond the NLO expressions. Considering the steepness of the chiral extrapolation in the light quark mass due to the chiral logarithms in Eqs. (28)–(30), we expect this to be the most important source of uncertainty. Indeed, this is generally confirmed by our fits showing a clear trend toward better fit qualities for stricter M_π cuts. Additionally, we apply a cut excluding the data at the coarsest lattice

spacing $a < a^{\text{cut}} = 0.08$ fm, as well as a cut in the lattice volume $L < L^{\text{cut}} = 3.5$ fm. Moreover, the fits have been carried out for all possible combinations of these data cuts. Combined with the variations in the previous analysis steps, there is a total number of $N_M = 910$ different models for the extrapolation of each of the three radii. In order to avoid fit stability issues that may arise for a few models with particularly small numbers of degrees of freedom $N_{\text{dof}} \sim 4$ on some of the bootstrap samples, a prior has been put on f_0 , i.e., the central value from the latest FLAG estimate [14] $f_0^{\text{prior}} = \sqrt{2}F_0^{\text{FLAG}} = 113.6$ MeV with a very broad width of 50%.

Figure 7 shows examples for the physical extrapolation of $\langle r_S^2 \rangle_\pi^0$ and $\langle r_S^2 \rangle_\pi^8$ as a function of the light and strange quark mass proxies as well as a^2 . Similarly, results for $\langle r_S^2 \rangle_\pi^l$ are shown in Fig. 8. Note that the respective figures for $\langle r_S^2 \rangle_\pi^0$, $\langle r_S^2 \rangle_\pi^8$, and $\langle r_S^2 \rangle_\pi^l$ are based on different input data sets (cuts) and have been selected to be representative of the final results for the radii obtained from the model average discussed in the next section. More specifically, the selected fits have been chosen such that they exhibit the

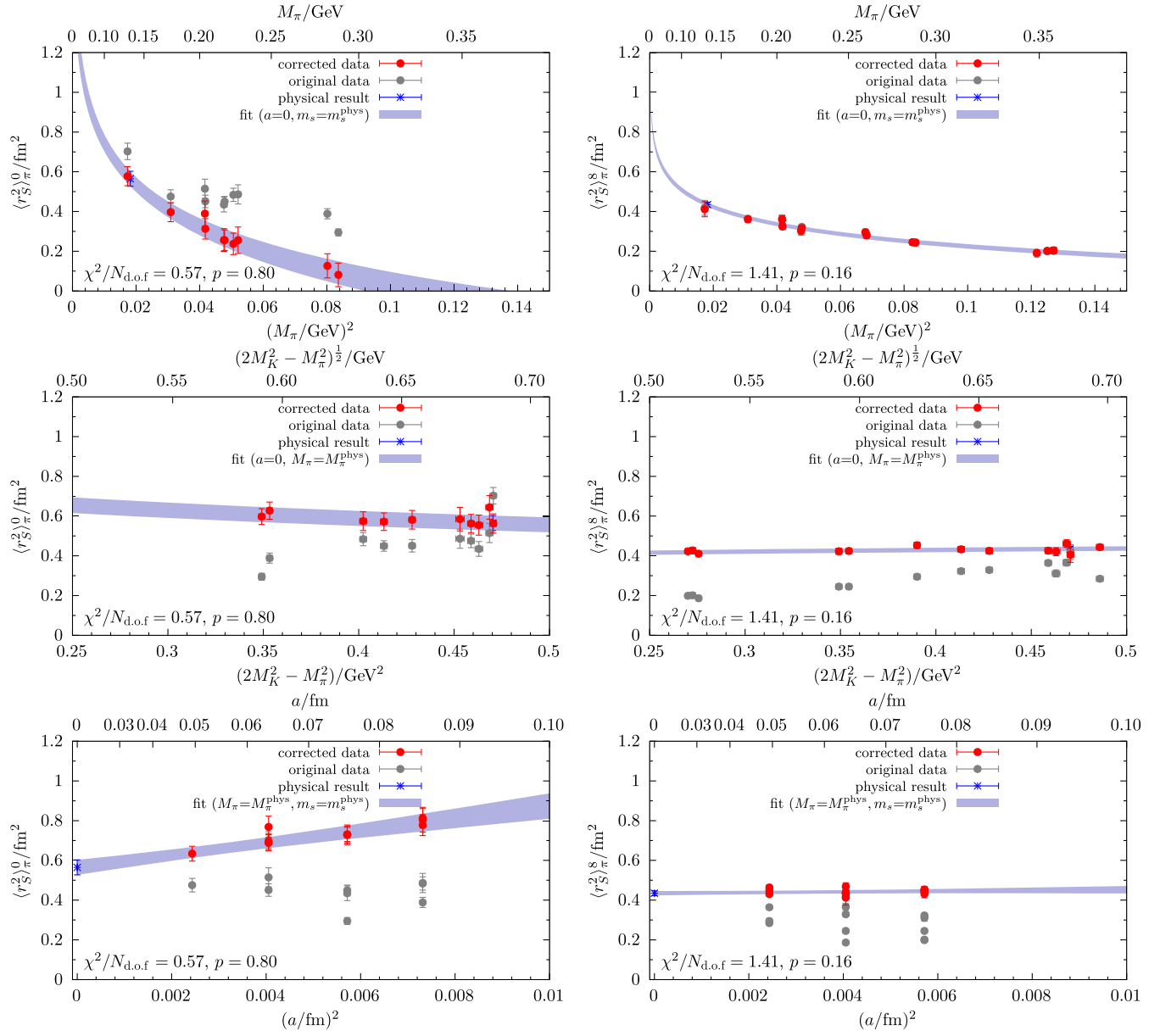


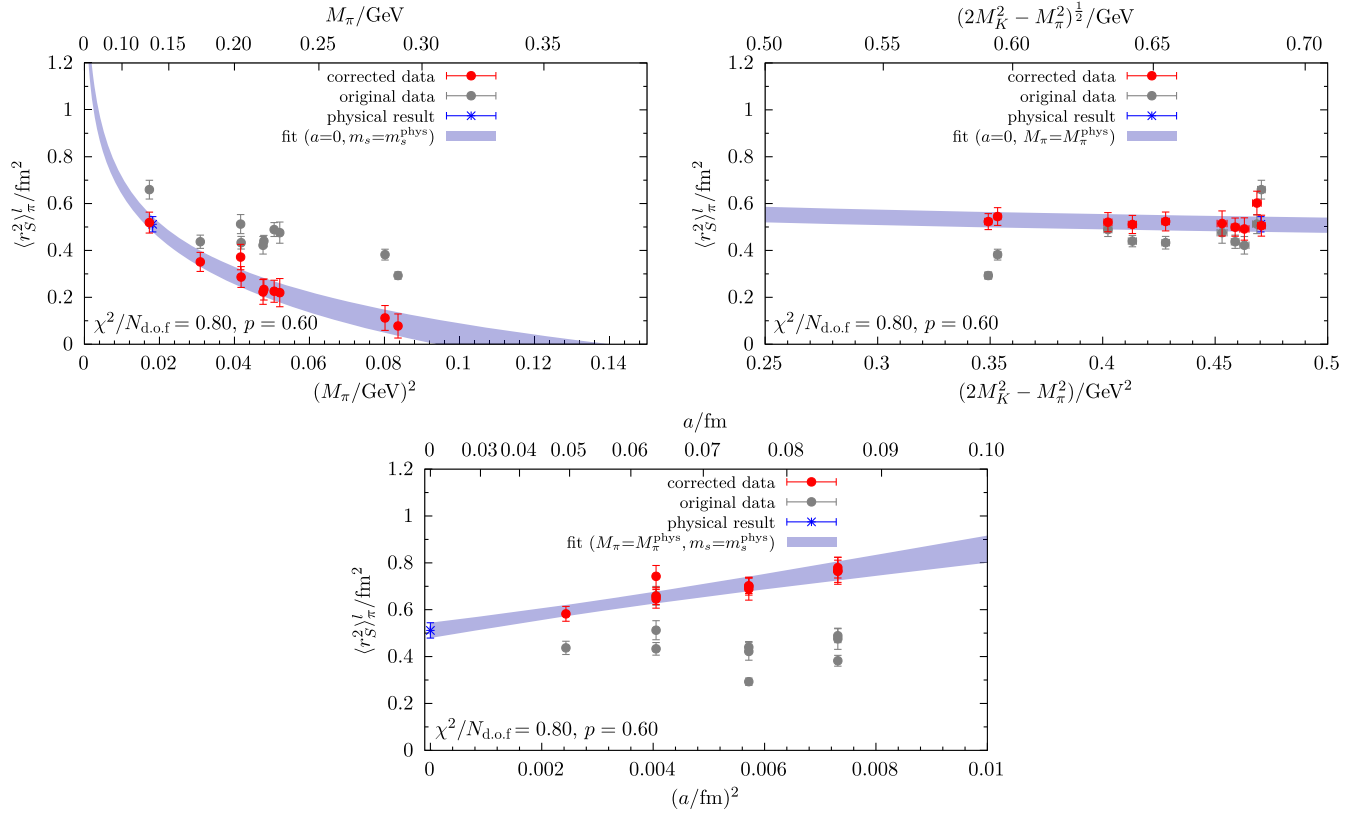
FIG. 7. Examples for the physical extrapolation of $\langle r_S^2 \rangle_\pi^0$ (left column) and $\langle r_S^2 \rangle_\pi^8$ (right column). The three figures for each observable show the extrapolation in the light and strange quark mass proxies M_π^2 and $2M_K^2 - M_\pi^2$, as well as the continuum limit are obtained from the same fit. Red (corrected) data are extrapolated to the physical point in all fit variables except the one shown on the horizontal axis, using parameters from the global fit.

largest weight, while their physical result for the radius is within one standard deviation of the statistical error of the final result.

First of all, our lattice data clearly reproduces the expected slope in M_π^2 due to the presence of the corresponding chiral logs in Eqs. (28)–(30). In particular, this trend is confirmed by the most chiral ensemble E250 with slightly lighter-than-physical light quark mass. Corrections due to the continuum limit are generally non-negligible as well for $\langle r_S^2 \rangle_\pi^0$ and $\langle r_S^2 \rangle_\pi^l$, whereas they tend to be smaller for $\langle r_S^2 \rangle_\pi^8$. However, we find that they can only be resolved

reliably in the presence of data cuts in the pion mass. This can be taken as another hint that higher order effects become relevant for $M_\pi \gtrsim 250$ MeV. A common feature of all three radii is that the chiral extrapolation in the strange quark mass is flat and essentially compatible with a constant. This feature remains very stable under data cuts.

Finally, concerning possible finite volume effects, we have tested several approaches. Unlike data cuts in M_π , there is no clear picture for cuts in L (or a). While a cut in L can still have some effect when combined with other cuts, there is no systematic trend observed. Furthermore, there is

FIG. 8. Same as Fig. 7 but for $\langle r_S^2 \rangle_\pi^I$.

no analytical expression for the finite size corrections to the pion scalar form factor available in the literature. However, we have tested the effect of adding corrections of the same form as the ones derived for meson masses and decay constants in Ref. [39], i.e., performing a simple substitution of the chiral logarithms

$$\log(t_0 M_P^2) \rightarrow \log(t_0 M_P^2) + \tilde{g}_1(M_P L), \quad P = \pi, K, \quad (31)$$

where $\tilde{g}_1(M_P L)$ is the function defined in Eq. (12) of Ref. [39]. Somewhat surprisingly, this leads quite consistently to slightly worse p values, whereas the resulting change to the physical values of the radii typically remains within the statistical uncertainty. Therefore, we refrain from including these variations into our final model averages. Furthermore, we have attempted to include a generic term of the form $\sim \tilde{g}_1(M_P L)$ with a free parameter as a coefficient. For the latter, we find that our data is not statistically precise enough to reliably disentangle such a term. In particular, for models involving fewer input data due to the aforementioned cuts, this often leads to unrealistically large, (anti)correlated cancellations with other terms and unstable fits. At any rate, we conclude that there is no obvious finite-size trend in our data at the current level of precision.

For the determination of the individual LECs L_4^r and L_5^r , it is convenient to fit suitable linear combinations of $\langle r_S^2 \rangle_\pi^I$,

$\langle r_S^2 \rangle_\pi^I$ and $\langle r_S^2 \rangle_\pi^8$ that give direct access to L_4^r and L_5^r as listed in Table IV. In particular, L_4^r is readily extracted, e.g., from the difference $\langle r_S^2 \rangle_\pi^0 - \langle r_S^2 \rangle_\pi^I$ as it parametrizes a pure strange quark effect mediated by the quark-disconnected contribution. Again, a term $\sim a^2/t_0$ is added to every fit model to account for scaling artifacts. As for the individual radii, these fits are carried out for all cuts and variations of the input data as well, which is reflected by the number of models N_M in Table IV. Note that the pion decay constant f_0 in the SU(3) chiral limit is obtained from any such fit model, as it only appears in a global prefactor in Eqs. (28)–(30). We remark that we have also attempted simultaneous fits to the data for all three radii. While such fits inherently

TABLE IV. List of fit models used to extract each of the pertinent SU(3) χ PT LECs, i.e., linear combinations of the expressions given through Eqs. (28)–(30). The number of fit models N_M also includes any further variations and (combinations of) data cuts at every stage of the analysis.

LEC	Fit models	N_M
f_0	$\langle r_S^2 \rangle_\pi^0, \langle r_S^2 \rangle_\pi^I, \langle r_S^2 \rangle_\pi^8, \langle r_S^2 \rangle_\pi^0 - \langle r_S^2 \rangle_\pi^I, \langle r_S^2 \rangle_\pi^0 - \langle r_S^2 \rangle_\pi^8, \langle r_S^2 \rangle_\pi^I - \langle r_S^2 \rangle_\pi^8$	5460
L_4^r	$\langle r_S^2 \rangle_\pi^0 - \langle r_S^2 \rangle_\pi^I, \langle r_S^2 \rangle_\pi^0 - \langle r_S^2 \rangle_\pi^8, \langle r_S^2 \rangle_\pi^I - \langle r_S^2 \rangle_\pi^8$	2730
L_5^r	$\langle r_S^2 \rangle_\pi^8, 3\langle r_S^2 \rangle_\pi^I - 2\langle r_S^2 \rangle_\pi^0$	1820

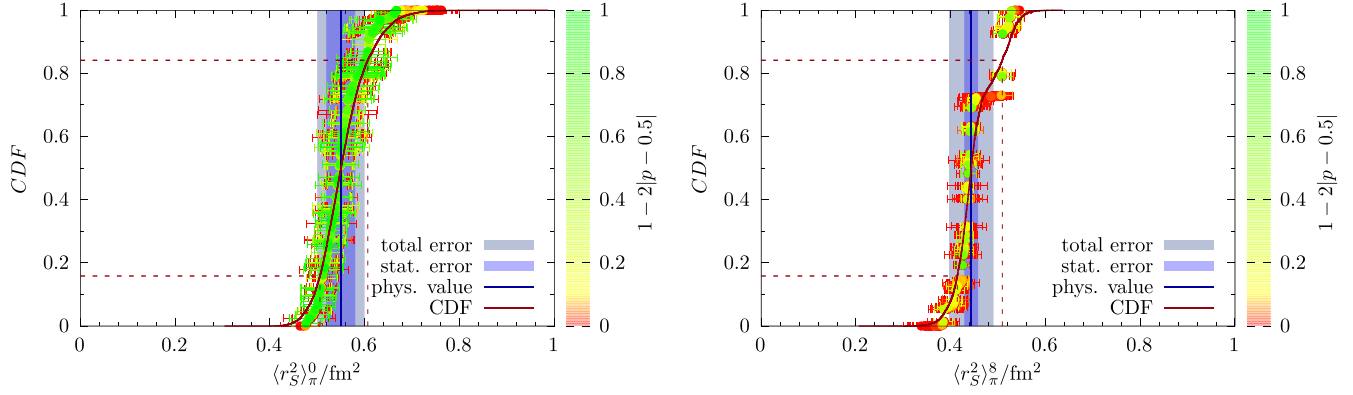


FIG. 9. Cumulative distribution functions (CDFs) of the results for the singlet and octet scalar radii $\langle r_S^2 \rangle_\pi^0$ and $\langle r_S^2 \rangle_\pi^8$. Each data point represents the result and statistical error from an individual fit model, and its color is determined by the corresponding p value weight indicating the quality of the fit. Note that the later is different from the Akaike weight actually used to obtain the CDF. The solid blue line indicates the final result from the model average and together with its statistical and full error bands. The dashed lines correspond to the 1σ quantiles of the CDF.

disentangle the contributions of individual LECs, they turn out to be problematic due to very strong correlations in the data resulting in a poorly estimated covariance matrix and typically unacceptable fit qualities.

VII. MODEL AVERAGES AND FINAL RESULTS

The individual results for the physical radii and LECs are combined in model averages to compute the final results with a full error budget. Taking into account the number of bootstrap samples, there are $\mathcal{O}(10^6)$ fits per observable. For each of these observables, we assign weights [40–42] to the respective models with index $n \in \{1, \dots, N_M\}$ and bootstrap sample $b \in \{1, \dots, N_B\}$,

$$w_{n,b} = \frac{e^{-B_{n,b}}}{\sum_{k=1}^{N_M} e^{-B_{k,b}}}. \quad (32)$$

These weights are based on a variation of the Akaike information criterion (AIC) [43,44], viz. the Bayesian AIC (BAIC) as introduced in Ref. [42],

$$B_{n,b} = \frac{1}{2} \chi_{n,b}^2 + N_{\text{par},n} + N_{\text{cut},n} - N_{\text{prio},n}, \quad (33)$$

where $\chi_{n,b}^2$ is the minimized, correlated χ^2 obtained from the n th fit model on the b th bootstrap sample. $N_{\text{par},n}$ and $N_{\text{cut},n}$ denote the numbers of fit parameters and data removed by cuts for the respective model. Finally, the number of priors $N_{\text{prio},n}$ is always the same; i.e., $N_{\text{prio},n} = 1$ because the fits do not require any priors besides the one on f_0 that is always present. For each observable O , we define the cumulative distribution function (CDF)

$$\text{CDF}(y) = \frac{1}{N_B} \sum_{n=1}^{N_M} \sum_{b=1}^{N_B} w_{n,b} \Theta(y - O_{n,b}), \quad (34)$$

where Θ is the Heaviside step function. Note that the CDFs are constructed in a fully nonparametric way, i.e., by directly using the bootstrap distributions, which differs from the approach discussed in Ref. [45] that relies on (weighted) Gaussian CDFs derived only from the central values and errors of the individual models. The median and the quantiles that correspond to 1σ errors for a Gaussian distribution define the central value and total error of the final results, respectively. Moreover, the total error is subdivided into a statistical and systematic contribution by a procedure similar to the one introduced in Ref. [45]. The only required modification is that the direct rescaling of the statistical errors has to be replaced by a rescaling of the widths of the bootstrap distributions in our approach. For the rescaling factor, we choose $\lambda = 2$.

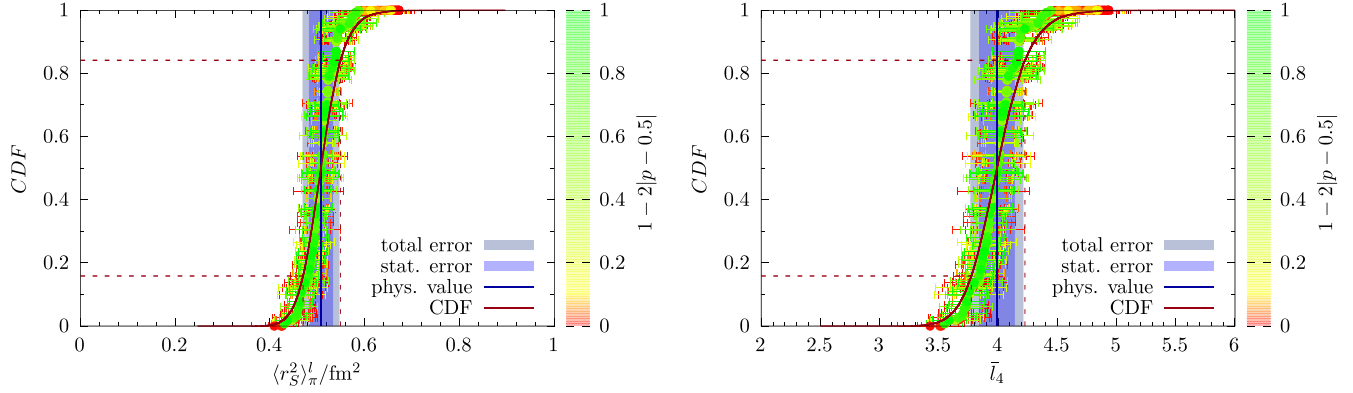
Figure 9 shows the CDFs and results for $\langle r_S^2 \rangle_\pi^0$ and $\langle r_S^2 \rangle_\pi^8$. The CDF for $\langle r_S^2 \rangle_\pi^0$ is in agreement with the assumption of Gaussian-distributed model data, whereas some skewness is observed for $\langle r_S^2 \rangle_\pi^8$. However, the data for the latter is statistically much more precise due to the (relative) smallness and precision of the $l-s$ quark-disconnected contribution, which is reflected by worse fit qualities for the individual models and results in an increased systematic error. The CDF for $\langle r_S^2 \rangle_\pi^l$ is shown in the left panel of Fig. 10 and is fairly similar to the one for $\langle r_S^2 \rangle_\pi^0$ concerning its shape and overall fit qualities of the underlying data, as expected. Our final results for the physical values of the three radii read

$$\langle r_S^2 \rangle_\pi^0 = 0.550(32)_{\text{stat}}(39)_{\text{sys}}[50]_{\text{total}} \text{ fm}^2, \quad (35)$$

$$\langle r_S^2 \rangle_\pi^l = 0.508(27)_{\text{stat}}(29)_{\text{sys}}[39]_{\text{total}} \text{ fm}^2, \quad (36)$$

$$\langle r_S^2 \rangle_\pi^8 = 0.443(16)_{\text{stat}}(45)_{\text{sys}}[47]_{\text{total}} \text{ fm}^2, \quad (37)$$

where the systematic error comprises a full error budget, i.e., the residual uncertainty due to excited states,

FIG. 10. Same as Fig. 10 but for $\langle r_S^2 \rangle_\pi^I$ and the closely related LEC $\bar{\ell}_4$.

form-factor parametrization and the physical-point extrapolation. Comparing these results to the only other available LQCD calculation involving strange quarks in Ref. [35], we find that our results are larger but in individual agreement within errors. The two-flavor calculation in Refs. [25,34], on the other hand, predicts a value for $\langle r_S^2 \rangle_\pi^I$ that is about 2σ larger than ours. This could readily be explained by the effect of the strange quark contribution, but we stress that our present calculation also exhibits much better control over various systematic effects.

The $\bar{\ell}_4$ LEC in SU(2) χ PT is directly related to $\langle r_S^2 \rangle_\pi^I$ via Eq. (6), which leads to a fairly similar shape for its CDF in the right panel of Fig. 10. The final result is given by

$$\bar{\ell}_4 = 3.99(15)_{\text{stat}}(17)_{\text{sys}}[23]_{\text{total}}, \quad (38)$$

where we have used $f_{\pi,\text{phys}} = 130.2(1.2)$ MeV from Ref. [46] as input to evaluate the rhs of Eq. (6). The value is in excellent agreement with the most recent FLAG estimate [14] $\bar{\ell}_4^{\text{FLAG}} = 4.02(45)$ for $N_f = 2 + 1$ flavors, but with only half the total error. Besides, our result is the first LQCD determination of $\bar{\ell}_4$ with $N_f = 2 + 1$ flavors from a form factor calculation, whereas all previous LQCD results [47–51] that enter the FLAG average are derived from decay constant calculations based on meson two-point functions. Finally, our result is in broad agreement with phenomenological analyses in, e.g., Refs. [52–55], although their results show a trend toward $\bar{\ell}_4 > 4$.

For the SU(3) LECs f_0 , L_4^r , and L_5^r , the final results are based on the models in Table IV, which is reflected by the larger number of data points in Fig. 11. For the pion decay constant in the SU(3) chiral limit, we find

$$f_0 = 116.5(5.5)_{\text{stat}}(13.7)_{\text{sys}}[14.8]_{\text{total}} \text{ MeV}, \quad (39)$$

which agrees with the FLAG value [14,47] $f_0 = 114.0(8.5)$ MeV, whereas a more recent study by the χ QCD collaboration in Ref. [56] prefers a much smaller value of $f_0 = 82.3(0.7)(14.1)$ MeV in stark contrast to our

result. Another recent study by the RQCD collaboration found [57] $f_0 = 99_{-3}^{+4}$ MeV. On the other hand, our value for f_0 agrees almost exactly with the semiphenomenological result $f_0 = 116.46(96)$ MeV in Ref. [58] from a N³LO global fit of octet and decuplet baryon masses on the CLS ensembles.

Results for the NLO LECs are commonly evaluated at a reference scale of $\mu = 770$ MeV, cf. Ref. [14]. Therefore, the fit results obtained from the physical extrapolation $L_{4,5}^{\text{fit}} = L_{4,5}(\mu = 1/\sqrt{t_0})$ are run to the reference scale via [2,59]

$$L_4^r(\mu) = L_4^{\text{fit}} - \frac{1}{256\pi^2} \log(t_0\mu^2), \quad (40)$$

$$L_5^r(\mu) = L_5^{\text{fit}} - \frac{3}{256\pi^2} \log(t_0\mu^2). \quad (41)$$

The final results from the model average read

$$L_4^r(\mu = 770 \text{ MeV}) = +0.38(09)_{\text{stat}}(15)_{\text{sys}}[18]_{\text{total}} \times 10^{-3}, \quad (42)$$

$$L_5^r(\mu = 770 \text{ MeV}) = +0.58(0.38)_{\text{stat}}(1.08)_{\text{sys}}[1.14]_{\text{total}} \times 10^{-3}. \quad (43)$$

Our determination for L_4^r is the first with controlled systematics and sufficient statistical precision to obtain a nonzero value. Furthermore, it is the only direct determination based on a form factor calculation. The only other two lattice results $L_4^r(\mu = 770 \text{ MeV}) = -0.02(56) \times 10^{-3}$ ($N_f = 2 + 1$, from Ref. [47]) and $L_4^r(\mu = 770 \text{ MeV}) = +0.09(34)$ ($N_f = 2 + 1 + 1$, from Ref. [60]) are compatible within errors but do not even agree on a common sign. Unlike for L_4^r , we find that our fits are not particularly sensitive to L_5^r , resulting in a rather substantial model spread in the lower panel of Fig. 11. This results in a significantly increased total error that is dominated by systematic uncertainty. However, the central value has the

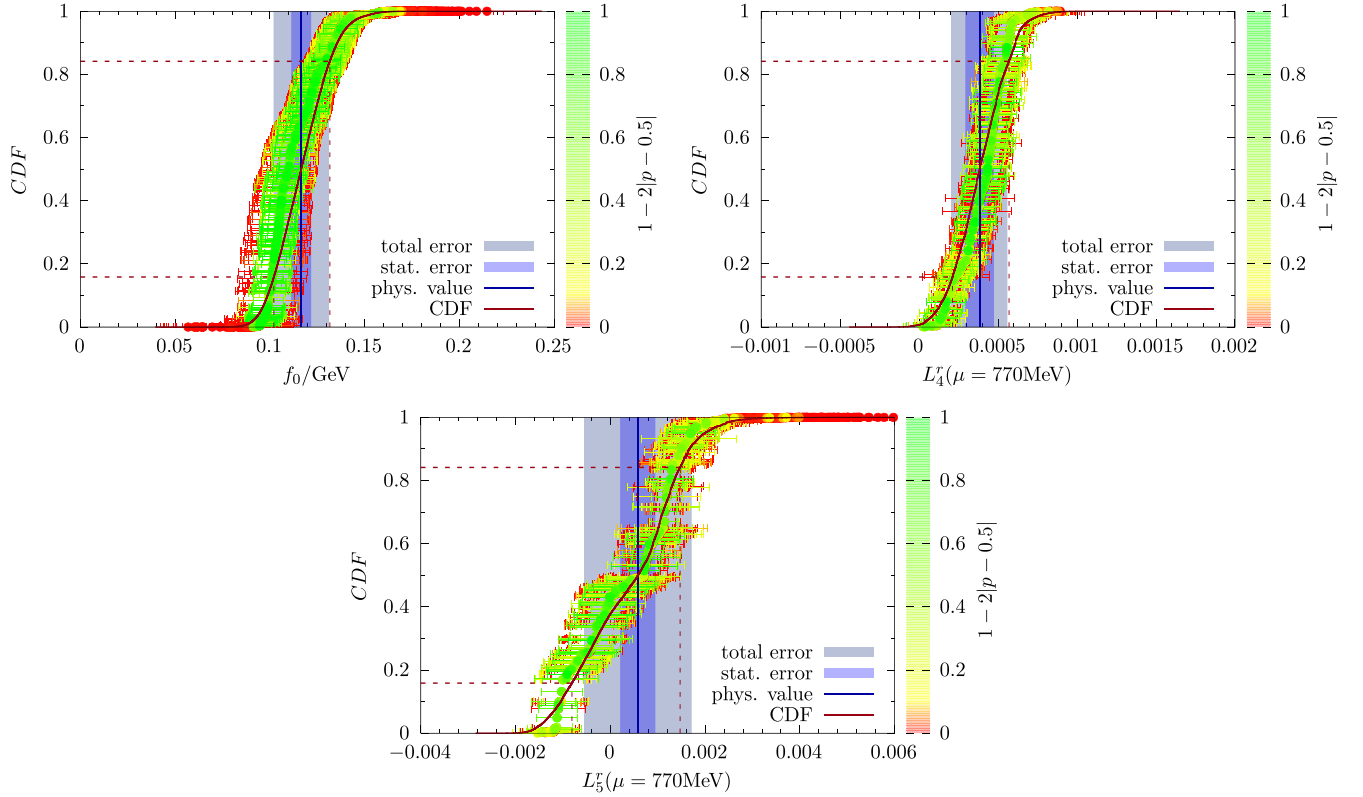


FIG. 11. Same as Fig. 10 but for the SU(3) LECs f_0 , $L_4^r(\mu)$ and $L_5^r(\mu)$ at a scale of $\mu = 770$ MeV.

correct sign and roughly same magnitude as other lattice determination from decay constant fits; cf. Refs. [47,60].

VIII. SUMMARY AND OUTLOOK

In this study, we have computed physical results for the pion scalar radii $\langle r_S^2 \rangle_\pi^0$, $\langle r_S^2 \rangle_\pi^8$, and $\langle r_S^2 \rangle_\pi^I$, as well as the pertinent LECs in the respective NLO expressions in SU(2) and SU(3) χ PT. The results feature a full error budget covering the systematic uncertainties at every stage of the analysis. This was made possible mainly by calculating the quark-disconnected contributions to $F_S^{\pi,f}(Q^2)$ with unprecedented statistical precision and momentum resolution. For the first time, this enabled us to, e.g., extract the pion scalar radii from a parametrization of the form factors beyond a simple, linear interpolation, and to obtain a nonzero result for L_4^r that depends entirely on the quark-disconnected contribution of the strange quark. Besides, our calculation confirms the importance of the quark-disconnected contribution for the pion scalar radius as predicted in Ref. [61] from a χ PT analysis. Furthermore, the statistical precision of the lattice data is mirrored by our result for the SU(2) LEC $\bar{\ell}_4$, which crucially depends on the light quark-disconnected contribution to the form factor. Lastly, our calculation confirms the observation in Refs. [34,35] that the quark-disconnected contribution to $F_S^{\pi,f}(Q^2)$ is affected by large lattice artifacts in the case of Wilson fermions.

In the future, it might be interesting to include additional ensembles at physical quark mass and even finer lattice spacing to further reduce systematic errors. Besides, since we have also computed and stored all local and one-link displaced insertion operators for the quark-connected three-point function, our calculation could rather easily be extended to further observables, such as, e.g., the pion and kaon vector radii and average quark momentum fractions.

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NHR (www.nhr-verein.de/unsere-partner). Additional calculations have been performed on the HPC clusters Clover at the Helmholtz-Institut Mainz, and Mogon II and HIMster-2 at Johannes-Gutenberg Universität Mainz. The QDP++ library [64] and the deflated SAP + GCR solver from the openQCD package [65] have been used in our simulation code. We thank our colleagues in the CLS initiative for sharing gauge ensembles.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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