

# Higher-order hadronic-vacuum-polarization contribution to the muon $g - 2$ from lattice QCD

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We calculate the  $O(\alpha^3)$  hadronic-vacuum-polarization contribution to the muon anomalous magnetic moment for the first time from *ab initio* lattice QCD. We employ previously-published results for the Taylor coefficients of the renormalized vacuum polarization function that were obtained on four-flavor QCD gauge-field configurations with physical light-quark masses. We obtain  $10^{10} a_\mu^{\text{HVP,HO}} = -9.3(1.3)$ , in agreement with determinations from  $e^+e^- \rightarrow \text{hadrons}$  data plus dispersion relations. The total uncertainty is below the target precision of the Muon  $g - 2$  Experiment. We also provide new expressions suitable for computing the  $O(\alpha^3)$  hadronic vacuum polarization contributions from the renormalized vacuum polarization function  $\hat{\Pi}(q^2)$ , or directly from the lattice vector-current correlator in Euclidean space.

## I. INTRODUCTION

The anomalous magnetic moment of the muon ( $g_\mu - 2$ ) is one of the most precisely-determined observables in particle physics, having been measured with an uncertainty of 0.54 parts-per-million by BNL Experiment E821 [1]. Because of this high experimental precision, and because the anomaly is mediated by quantum-mechanical loops in the Standard Model, the muon  $g_\mu - 2$  provides stringent constraints on new heavy or weakly-coupled particles. The present Standard-Model theory value lies below the BNL E821 measurement by more than three standard deviations [2]. To identify definitively whether this deviation is due to new particles or forces, both the theory and measurement errors must be improved. The Muon  $g_\mu - 2$  Experiment recently began running at Fermilab, and aims to reduce experimental error by a factor of four [3]. In parallel, numerous efforts are underway by the lattice-QCD community to tackle the Standard-Model hadronic contributions [4–13], which are the largest source of theory uncertainty [2].

The largest source of uncertainty in the Standard-Model  $g_\mu - 2$  is from the  $O(\alpha^2)$  hadronic vacuum-polarization (HVP) contribution [2],  $a_\mu^{\text{HVP}}$ , which is shown in Fig. 1.<sup>1</sup> This contribution can be obtained by combining experimental measurements of electron-positron inclusive scattering into hadrons with dispersion relations, and recent determinations from this approach quote errors of 0.4–0.6% [14–16]. The most precise calculation of the leading-order  $a_\mu^{\text{HVP}}$  to-date from Ref. [8] employed four-flavor lattice QCD with physical-

mass pions to achieve a total error of  $\sim 2\%$ . A significant source of systematic uncertainty in this and all lattice-QCD results to-date is from the use of degenerate up- and down-quark masses; phenomenological estimates of this error are about 1% [17–19]. Recently, we calculated the strong-isospin-breaking correction to the leading-order, light-quark-connected contribution to  $a_\mu^{\text{HVP}}$  directly for the first time with the physical values of  $m_u$  and  $m_d$ , thereby removing this important uncertainty contribution [20]. To match the target experimental precision, however, the error on  $a_\mu^{\text{HVP}}$  must be further reduced to about 0.2%.

The  $O(\alpha^3)$  “higher-order” hadronic vacuum-polarization contribution to  $g_\mu - 2$  is roughly 1.5% that of the leading-order HVP contribution [2], and therefore only needs to be determined to around 10% to match the projected experimental precision. Experimental determinations from combining electron-positron inclusive scattering into hadrons data with dispersion relations quote errors of 0.4–0.9% [14, 16, 21]. Nevertheless, it is important to check these phenomenological values with *ab-initio* QCD calculations. Moreover, if the disagreement between theory and experiment persists or grows with the new Muon  $g_\mu - 2$  measurement, a complete first-principles Standard-Model theory value will be essential for drawing conclusions about the presence or nature of new physics.

In this paper we calculate the higher-order HVP contribution to  $a_\mu^{\text{HVP}}$  for the first time in lattice QCD. To enable us to focus on the methodology and error analysis, we use previously published lattice-QCD results for the Taylor coefficients of the renormalized vacuum polarization function ( $\hat{\Pi}(Q^2)$ ) from Refs. [8, 22–24] to construct both Padé [23] and Mellin-Barnes approximants [25] for  $\hat{\Pi}(Q^2)$ . Details on the lattice-QCD calculations can be found in these works.

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<sup>1</sup> The symbol  $\alpha$  always denotes the electromagnetic coupling in this work.

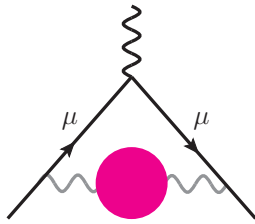


FIG. 1. Leading hadronic contribution to the muon  $g_\mu - 2$ . The shaded circle denotes all corrections to the internal photon propagator from the vacuum polarization of  $u$ ,  $d$ ,  $s$ ,  $c$ , and  $b$  quarks in the leading one-loop muon vertex diagram.

This paper is organized as follows. In Sec. II, we provide theoretical background on the hadronic-vacuum-polarization contributions to  $g_\mu - 2$ , and discuss our method for calculating the higher-order contributions. Next, in Sec. III we present our analysis and error budget. Last, in Sec. IV, we show our final result for  $a_\mu^{\text{HVP,HO}}$  and compare with non-lattice determinations. Appendix A provides expressions suitable for computing the  $\mathcal{O}(\alpha^3)$  hadronic vacuum-polarization contribution to  $a_\mu^{\text{HVP}}$  directly from lattice-QCD simulations, while App. B provides the definition of the  $N = 2 + 1 + 1$  Mellin-Barnes approximant for the  $\hat{\Pi}(Q^2)$  used in this paper. For completeness, App. C gives the values of the quark-connected Taylor coefficients employed in our analysis.

## II. THEORETICAL BACKGROUND

The leading hadronic contribution to the muon anomalous magnetic moment arises from QCD corrections to the internal photon propagator in the  $\mathcal{O}(\alpha^2)$  one-loop muon vertex diagram, as shown in Fig. 1. At  $\mathcal{O}(\alpha^3)$ , higher-order hadronic contributions arise from adding a second internal photon line (as in Fig. 2 (a)), adding a lepton loop to the existing photon line (as in Figs. 2 (a) and (b)), or adding a second insertion of the hadronic vacuum polarization bubble on the photon line (as in Fig. 2 (c)). Both the leading- and NLO HVP contributions can be obtained, with the help of dispersion relations, from the energy scan of the experimental “R-ratio” [14–16, 21]:

$$R_\gamma(s) \equiv \frac{\sigma(e^+e^- \rightarrow \gamma^* \rightarrow \text{hadrons})}{4\pi\alpha(s)^2/(3s)}, \quad (2.1)$$

where  $s$  is the square of the center-of-mass energy. Table I shows two recent evaluations of the leading contribution and the individual higher-order contributions from diagrams (a), (b), and (c) by Jegerlehner [14] and Keshavarzi *et al.* [16]. The higher-order contributions are roughly 1.5% of the leading contribution, and do not contribute substantially to the total error on the Standard-Model theory value for  $a_\mu$ .

Integrals for the  $\mathcal{O}(\alpha^3)$  contributions from diagrams (a)–(c) have been presented in the literature in terms of  $R_\gamma(s)$  [26, 27]. These formulations, however, are not

TABLE I. Determinations of the  $\mathcal{O}(\alpha^2)$  (first column) and  $\mathcal{O}(\alpha^3)$  hadronic-vacuum-polarization contributions (remaining columns) to  $g_\mu - 2$  from recent analysis of experimental data for the  $e^+e^- \rightarrow \text{hadrons}$  cross section by Jegerlehner [14] (top row) and Keshavarzi *et al.* [16] (bottom row).

Lowest order	$10^{10} a_\mu^{\text{HVP}}$			
	(a)	(b)	(c)	total HO
688.07(4.14)	-20.613(130)	10.349(63)	0.337(5)	-9.927(67)
693.27(2.46)	-20.77(8)	10.62(4)	0.34(1)	-9.82(4)

suitable for our use, particularly in the case of contribution (a). We therefore provide in Appendix A new expressions for these contributions that are amenable to use with lattice-QCD data. For each contribution, we provide two formulations to obtain  $a_\mu^{(i)}$ ;  $i = \{a, b, c\}$ . First, we use the following relationship between  $R_\gamma(s)$  and the renormalized vacuum polarization function [28],

$$\hat{\Pi}(q^2) = \frac{q^2}{3} \int_0^\infty ds \frac{R_\gamma(s)}{s(s+q^2)}, \quad (2.2)$$

to derive expressions in terms of the renormalized vacuum polarization function  $\hat{\Pi}(Q^2) \equiv \Pi(Q^2) - \Pi(0)$ .<sup>2</sup> These are the higher-order analogs of the original Blum formula for the leading HVP contribution [29], and are given in Eqs. (A1), (A6), and (A13). We also provide expressions for the contributions from diagrams (a)–(c) directly in terms of the Euclidean vector-current correlator at zero momentum  $G(t)$  using the relationship between  $\hat{\Pi}(Q^2)$  and  $G(t)$  below [28]:

$$\hat{\Pi}(\omega^2) \equiv 4\pi^2 (\Pi(\omega^2) - \Pi(0)) \quad (2.3)$$

$$= \frac{4\pi^2}{\omega^2} \int_0^\infty dt G(t) \left[ \omega^2 t^2 - 4 \sin^2 \left( \frac{\omega t}{2} \right) \right] \quad (2.4)$$

These are the higher-order analogs of the time-momentum representation formulated by Bernecker and Meyer for the leading HVP contribution, and are given in Eqs. (A3), (A11), and (A14).

The higher-order HVP contributions are sensitive to the value of the renormalized vacuum polarization function at larger values of  $Q^2$  than the leading-order contribution. Figure 3, left, plots the integrands for the leading-order and higher-order contributions as a function of  $Q^2$  using the  $N = 2 + 1 + 1$  Mellin-Barnes approximant for  $\hat{\Pi}(Q^2)$  from Ref. [25]. The integrand for the leading-order contribution is also shown for comparison. The integrand of contribution (a) has large positive and negative contributions below  $Q^2 = m_\mu^2$  that cancel substantially. Because of this, the large- $Q^2$  region is numerically important, with about 5% of the value of  $a_\mu^{(a)}$

<sup>2</sup> We use  $q^2$  and  $Q^2$  to denote the squared four-momenta in Minkowski and Euclidean space, respectively.

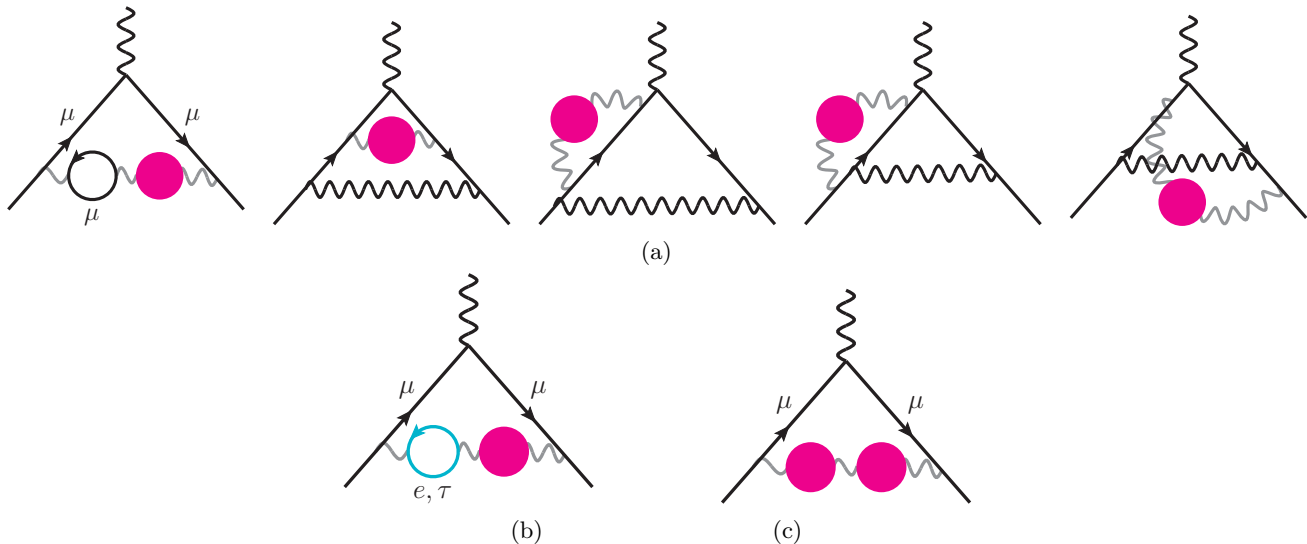


FIG. 2. Higher-order hadronic-vacuum-polarization contributions to  $g_\mu - 2$ . For contribution (a), diagrams that are reflections across the horizontal midpoint and diagrams in which the tree and corrected photon propagators are interchanged are not shown.

coming from  $Q^2 > 10\text{GeV}^2$ . The integrand of contribution (b) peaks around  $Q^2 = m_\mu^2/2\sqrt{2}$ , and more than 95% of the value of  $a_\mu^{(b)}$  comes from  $Q^2 < 0.5\text{GeV}^2$ . The integrand of contribution (c) peaks around  $Q^2 = 2m_\mu^2$ . Because it is proportional to  $\hat{\Pi}(Q^2)^2$ , it decreases less rapidly with  $Q^2$  than the other contributions; about 10% of the value of  $a_\mu^{(c)}$  comes from  $Q^2 > 1\text{GeV}^2$ . Thus, it is important to employ approximants of  $\hat{\Pi}(Q^2)$  that accurately reproduce the large- $Q^2$  behavior when calculating the higher-order contributions to  $a_\mu^{\text{HVP}}$ .

The higher-order HVP contributions are sensitive to the value of the Euclidean-time correlator at similar times as the leading-order contribution. Figure 3, right, plots the integrands for the leading-order and higher-order contributions (a) and (b) as a function of correlator time  $t$  using  $G(t)$  obtained from the spectral representation of  $R_\gamma(s)$ . (The kernel for contribution (c) depends upon the product of the correlator at two times  $G(t)G(t')$  and thus the integrand cannot be conveyed in a one-dimensional plot.) The leading-order (higher-order) kernels are proportional to  $t$  ( $t^2$ ) at small Euclidean times, and are proportional to  $1/t$  (approach a constant) at large times, and the integrands all peak at around  $t \sim 0.8\text{--}1.0$  fm. The contributions to  $a_\mu^{\text{HVP}}$  from correlator data beyond 4 fm, which is approximately half the temporal extent (or less) of lattices employed in recent  $g - 2$  calculations, are about 0.5% or less [8, 11, 12, 30].

### III. ANALYSIS

In this section we calculate the  $\mathcal{O}(\alpha^3)$  contributions to  $a_\mu^{\text{HVP}}$  from the diagrams in Fig 2. First, in Sec. III A, we describe the approximants of the renormalized vacuum

function used to calculate the higher-order HVP contributions. Next, we calculate the quark-connected contribution from light and heavy quarks in Sec. III B. Last, in Sec. III C, we estimate the size of the quark-disconnected contribution.

#### A. Approximants of $\hat{\Pi}(Q^2)$

We calculate the higher-order contributions to  $a_\mu^{\text{HVP}}$  using both Padé and Mellin-Barnes approximants of the renormalized vacuum polarization function in the QED integrals given in Appendix A. Both approaches employ the Taylor coefficients  $\Pi_i$  of  $\hat{\Pi}(Q^2)$  expanded about  $Q^2 = 0$ :

$$\hat{\Pi}(Q^2) = \sum_{i=1}^{\infty} \Pi_i Q^{2i} \quad (3.1)$$

As observed in Ref. [23], the  $\Pi_i$  are proportional to the time-moments of the vector-current correlation function, and can be computed with small statistical errors in lattice QCD. Further, with both the Padé and Mellin-Barnes approaches, only the first few Taylor coefficients are needed to obtain the leading-order HVP with a sub-percent systematic uncertainty associated with the parameterization of  $\hat{\Pi}(Q^2)$  [8, 25].

Following the method introduced by the HPQCD Collaboration [23], we construct the  $[n, m]$  Padé approximants for the renormalized hadronic vacuum polarization function from the  $\Pi_i$ 's. The true result for  $\hat{\Pi}(Q^2)$  is guaranteed to lie between the  $[n, n]$  and  $[n, n - 1]$  Padé approximants. For the leading-order HVP contribution, the Padé approximants provide a sufficiently accurate approximation of  $\hat{\Pi}(Q^2)$  both at low and high

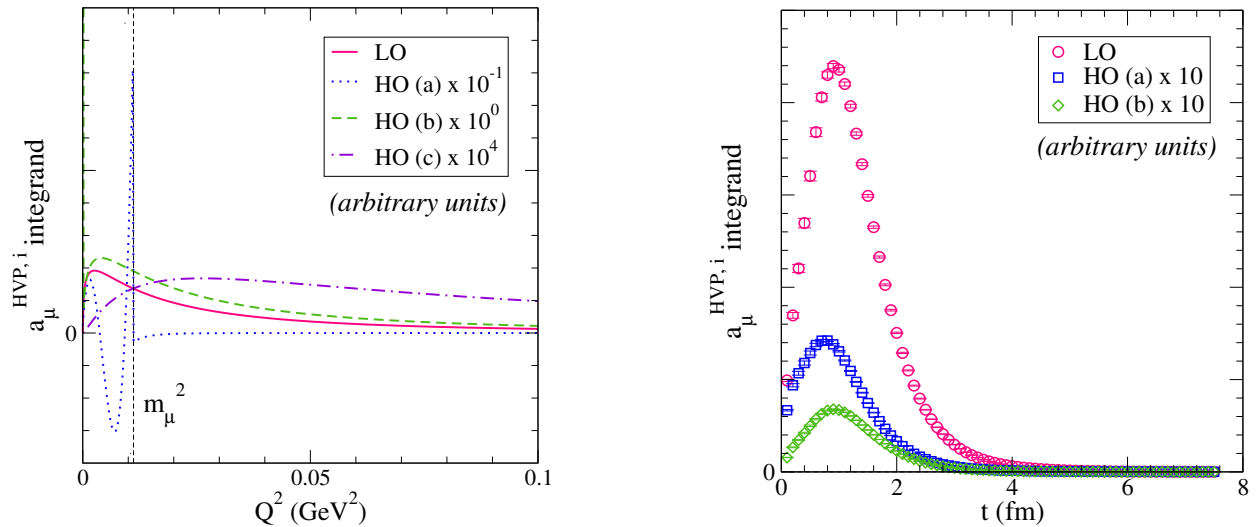


FIG. 3. (*color online.*) *Left:* integrands of Eqs. (A1) (blue dots), (A6) (green dashes), and (A13) (purple dot-dashes) obtained from the  $N = 2 + 1 + 1$  Mellin-Barnes approximant for  $\hat{\Pi}(Q^2)$  given in Ref. [25], which employs preliminary moments of  $R_\gamma(s)$  provided by Keshavarzi *et al.* [16]. The leading-order integrand is also shown as a solid magenta line for comparison. *Right:* integrands of Eqs. (A3) (blue squares) and (A11) (green diamonds) obtained from the parameterization of  $R_\gamma(s)$  provided by Jegerlehner in his public `alphaQED FORTRAN` package [31]. The leading-order integrand is also shown as magenta circles for comparison.

$Q^2$  that the associated uncertainty in  $a_\mu^{\text{HVP}}$  is below 1% by  $n = 2$  [8]. Unfortunately, however, one cannot use the  $[n, n-1]$  approximants  $\hat{\Pi}(Q^2)$  to calculate the contributions to  $a_\mu^{\text{HVP}}$  from diagrams (a) and (c). This is because  $\hat{\Pi}^{[n, n-1]}(Q^2) \sim Q^2$  as  $Q^2 \rightarrow \infty$ , making the integrals diverge in this limit. The integrals using the  $[n, n]$  Padé approximants are well behaved, but another approach is needed to quantify the uncertainty in the higher-order contributions to  $a_\mu^{\text{HVP}}$  from the parameterization of  $\hat{\Pi}(Q^2)$ .

Recently de Rafael and Charles *et al.* introduced the method of “Mellin-Barnes approximants” to obtain  $a_\mu^{\text{HVP}}$  from the Taylor coefficients of  $\hat{\Pi}(Q^2)$  [25, 32]. This approach uses the fact that the hadronic spectral function  $\text{Im}\hat{\Pi}(q^2)/\pi$  in QCD is positive and approaches a constant as  $Q^2 \rightarrow \infty$  to identify a class of functions that can be employed as successive approximants to the Mellin transform  $\mathcal{M}(s)$  of the hadronic spectral function. Given  $N$  moments of the Mellin transform  $\mathcal{M}(-n)$ , the Mellin-Barnes approximant  $\mathcal{M}_N$  smoothly interpolates between these known values, and approaches the asymptotic value of  $\mathcal{M}(s)$  from leading-order perturbative QCD as  $s \rightarrow \infty$ . The Mellin moments are trivially related to the Taylor coefficients of  $\hat{\Pi}(Q^2)$  as

$$\mathcal{M}(-n) = 4\pi\alpha(-1)^n(4m_\pi^2)^{(n+1)}\Pi_{n+1}, \quad (3.2)$$

The first term in the moment expansion of the hadronic spectral function provides a rigorous upper bound on  $\hat{\Pi}(Q^2)$  and  $a_\mu^{\text{HVP}}$  [33]. In practice, the  $N = 1$  approximant obtained using  $\mathcal{M}(0)$  from experimental  $R_\gamma$  data yields a value for the leading-order HVP contribution

that already agrees with the full result to better than 1% [25].

Figure 4 plots the Padé and Mellin-Barnes approximants for  $\hat{\Pi}(Q^2)$  calculated from the first four moments of  $R_\gamma(s)$  [16], and compares them with the exact result obtained from direct integration of  $R_\gamma(s)$ . The Mellin-Barnes approximants are closer to the exact  $\Pi(Q^2)$  than the Padés because they are constrained to satisfy the asymptotic perturbative-QCD behavior as  $Q^2 \rightarrow \infty$ . Note, however, that the rate at which the Mellin-Barnes approximants approach the true  $\hat{\Pi}(Q^2)$  depends upon the specific functional form employed at each order. In particular, the difference between successive approximants is not guaranteed to decrease with increasing  $N$ .

## B. Quark-connected contribution

We calculate the  $\mathcal{O}(\alpha^3)$  quark-connected contribution to  $a_\mu^{\text{HVP}}$  using the Taylor coefficients of  $\hat{\Pi}(Q^2)$  obtained by the HPQCD Collaboration in Refs. [8, 22–24]. The  $u$ ,  $d$ , and  $s$ -quark Taylor coefficients were calculated on the MILC Collaboration’s QCD four-flavor gauge-field configurations with highly-improved staggered (HISQ) sea and valence quarks [35, 36]. The  $b$ -quark Taylor coefficients were also calculated on the HISQ ensembles, but with a radiatively-improved nonrelativistic QCD action for the  $b$  quarks [37, 38]. The  $c$ -quark Taylor coefficients were calculated with HISQ valence quarks, but on MILC’s three-flavor ensembles with asqtad sea quarks [39–41]. The MILC ensembles are isospin-symmetric, *i.e.* the up and down sea-quark masses are

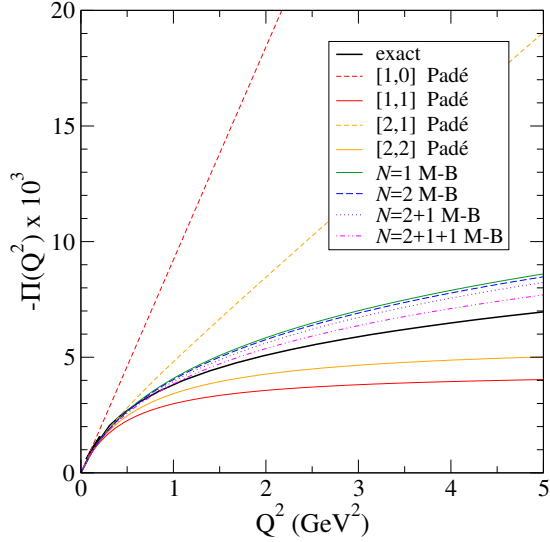


FIG. 4. (color online.) First four Padé approximants (“[1,0]–[2,2] Padé”) and Mellin-Barnes approximants (“N=1–N=2+1+1 M-B”) of the renormalized vacuum polarization function calculated from the moments of  $R_\gamma(s)$  analysis of Keshavarzi *et al.* [16] and quoted in Ref. [25]. The exact result is shown as a solid black line for comparison [34].

degenerate. The light-quark mass varies from  $m_l = m_s/5$  to Nature’s value  $m_l \sim m_s/27$ , making a chiral extrapolation unnecessary, and the strange- (and charm-) sea-quark masses are fixed to close to their physical values.

We employ light- and strange-quark Taylor coefficients on two ensembles with physical light-quark masses and lattice spacings  $a \approx 0.15$  fm and 0.12 fm from Refs. [8, 23]. Table IV gives the light- and strange-quark connected Taylor coefficients used in our analysis. The values of  $\Pi_i^{(ud)}$  include corrections for the finite lattice spatial volume and nonzero lattice spacing computed at one-pion-loop order within scalar QED [18]. We employ charm- and bottom-quark Taylor coefficients from Refs. [22, 24], which provide values of  $\Pi_i^{(c)}$  and  $\Pi_i^{(b)}$  at the physical light-quark mass and in the continuum. For convenience, Table V gives the heavy-quark connected Taylor coefficients used in our analysis.

To calculate the connected contribution to  $a_\mu^{(\text{HO})}$ , we first sum the individual Taylor coefficients  $\Pi_i^{(ud)}$ ,  $\Pi_i^{(s)}$ ,  $\Pi_i^{(c)}$ , and  $\Pi_i^{(b)}$ , and then use the total to construct the Padé and Mellin-Barnes approximants for  $\hat{\Pi}(Q^2)$ . Beyond  $N = 2$ , the functional forms of the Mellin-Barnes approximants are not unique; Appendix B gives the form of  $\hat{\Pi}_{2+1+1}(Q^2)$  used here. We then use the resulting approximants for  $\hat{\Pi}(Q^2)$  in the QED integrals, Eqs. (A1), (A6), and (A13), to obtain the quark-connected contributions to  $a_\mu^{\text{HVP}}$  from the diagrams in Fig. 2. On each ensemble, and for each contribution (a)–(c), we average the values from the Padé and Mellin-Barnes approximants, and take half the difference between the two as the systematic uncertainty from the parameterization of  $\hat{\Pi}(Q^2)$ .

TABLE II.  $\mathcal{O}(\alpha^3)$  hadronic-vacuum-polarization contributions to  $g_\mu - 2$  on two physical-mass HISQ ensembles obtained using [2,2] Padé and  $N = 2 + 1 + 1$  Mellin-Barnes approximants for  $\hat{\Pi}(Q^2)$ . The uncertainties are from the errors on the Taylor coefficients and, for the averages, from the use of approximants for  $\hat{\Pi}(Q^2)$ .

$\approx a$ (fm)	$\hat{\Pi}$ approx.	$10^{10} a_\mu^{\text{HO, conn.}}$		
		(a)	(b)	(c)
0.15	Padé	-19.24(32)	10.34(10)	0.3186(79)
	M-B	-20.82(35)	10.40(19)	0.339(12)
	Average	-20.03(82)	10.37(11)	0.329(12)
0.12	Padé	-19.05(29)	10.176(87)	0.3111(69)
	M-B	-20.58(27)	10.23(15)	0.3307(89)
	Average	-19.82(79)	10.204(91)	0.321(11)

Table II gives the results on the two ensembles employed in our analysis.

Figure 5 shows the total  $\mathcal{O}(\alpha^3)$  quark-connected contribution to  $a_\mu^{\text{HVP}}$  — obtained by summing contributions (a)–(c) in the rows labeled “average” in Table II — versus squared lattice spacing. The data do not display any significant lattice-spacing dependence, so we fit them to constant to obtain the continuum-limit value of  $a_\mu^{\text{HVP,HO}}$ . We also consider an alternative linear extrapolation in  $a^2$  to a function of the form

$$a_\mu^{\text{HVP,HO}} \left( 1 + c_{a^2} \frac{(a\Lambda)^2}{\pi^2} \right), \quad (3.3)$$

with  $\Lambda = 500$  GeV a typical QCD scale. The linear-fit result for  $c_{a^2}$  is consistent with zero, and for  $a_\mu^{\text{HVP,HO}}$  is close to the value from the constant fit. We therefore conclude that discretization effects are smaller than the fit error on  $a_\mu^{\text{HVP,HO}}$ , and do not assign a separate systematic error from this source.

The HPQCD Collaboration reduced the statistical errors in the light-quark connected Taylor coefficients in Ref. [8] by using fit results for the vector-current correlators for times greater than 1.5 fm. Although the lowest-energy states in these correlators are  $I = 1$   $\pi\pi$  pairs, no evidence of such states was seen in the two-point fits, and the ground-state energies obtained are consistent with the experimental  $\rho^0$  meson mass. HPQCD estimate the contribution to the leading-order light-quark connected contribution to  $a_\mu^{\text{HVP}}$  from the omitted  $\pi\pi$  states within scalar QED to be  $3 \times 10^{-10}$ . We expect  $\pi\pi$  contributions to be similar in size for the dominant higher-order diagrams (a) and (b) because the integrands in Eqs. (A1) and (A6) are proportional to  $\hat{\Pi}(Q^2)$ , just as for the leading-order hadronic vacuum polarization. Hence, we take the same percentage error of 0.5% as the uncertainty in  $a_\mu^{\text{HVP,HO}}$  from  $\pi\pi$  states below the  $\rho$  pole.

The four-flavor gauge-field ensembles employed in our analysis have degenerate up and down sea-quark masses. Recently the Fermilab Lattice, HPQCD, and MILC Col-



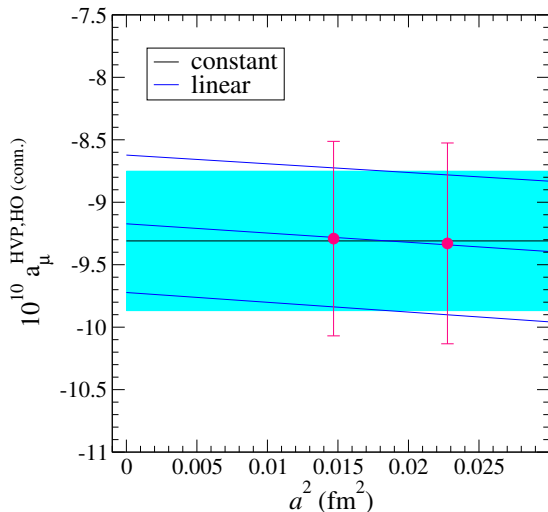


FIG. 5. (*color online.*) Continuum extrapolation of  $O(\alpha^3)$  quark-connected contribution to  $a_\mu^{\text{HVP}}$ . The filled cyan band shows the result of our preferred constant fit, while the solid blue lines show the result of a linear fit to Eq. (3.3) with the slope  $c_{a^2}$  constrained with a Gaussian prior  $0 \pm 1$ .

laborations calculated the strong-isospin-breaking correction to  $a_\mu^{\text{HVP}}$  for the first time with physical values  $m_u$  and  $m_d$  [20]. They obtain  $+1.5(7)\%$  for the relative correction that should be applied to the leading-order light-quark connected contribution, in agreement with phenomenological estimates [17–19]. Here we use  $+1.5(1.0)\%$  to correct the continuum-limit value of  $a_\mu^{\text{HVP,HO}}$  from Fig. 5, where we have taken a larger uncertainty of 1% on the relative correction to account for the fact that the shift was not calculated directly for the higher-order hadronic vacuum polarization.

The QCD gauge-field ensembles employed in our analysis do not include effects due to the quarks’ nonzero electromagnetic charges in Nature. The dominant QED effect in  $a_\mu^{\text{HVP}}$  arises from producing a hadron polarization bubble consisting of a  $\pi^0$ - $\gamma$  pair. Following Hagiwara *et al.* [42] we calculate the contribution to  $a_\mu^{\text{HVP,HO}}$  from  $e^+e^- \rightarrow \pi^0\gamma$  in the region  $0.6 < \sqrt{s} < 1.03$  GeV using the latest experimental data for this channel from the SND Experiment [43]. We obtain

$$\Delta a_\mu^{(\text{HO}, \pi^0\gamma)} = -0.056(8) \times 10^{-10}, \quad (3.4)$$

which is approximately 0.6% of the total quark connected contribution. We therefore take 1% as the error from the omission of electromagnetism in the simulations.

Finally, as discussed in Appendix A, in order to express higher-order contribution 2(a) in Fig. 1 in terms of the renormalized vacuum polarization function, we must drop terms in the original integrand [26, 27] that are proportional to  $(m_\mu^2/s)^n \log^2(m_\mu^2/s)$ . We have calculated the numerical size of these terms from experimental  $R_\gamma(s)$  data [31] and, although they are small, they are not negligible given the size of our statistical and other systematic

TABLE III. Error budget for  $O(\alpha^3)$  quark-connected contribution to  $g_\mu - 2$ .

	$a_\mu^{(\text{HO}, ud)}$ (%)
Omission of $\log^2$ terms	10.6
Padé approximants	5.8
Isospin-breaking and electromagnetism	1.4
Taylor coefficients	1.2
$\pi\pi$ states ( $t^*$ )	0.5
Total	12.2

uncertainties. To account for the omission of the “ $\log^2$ ” in our calculation of contribution 2(a) via Eq. (A1), we therefore include an additional systematic uncertainty of  $1 \times 10^{-10}$ , which is almost twice the size of these terms calculated from  $R_\gamma(s)$  data.

Table III gives the complete error budget for the  $O(\alpha^3)$  quark-connected contribution to  $a_\mu^{\text{HVP}}$ . The largest uncertainties are associated with the omitted “ $\log^2$ ” terms in contribution 2(a) and from the use of Padé and Mellin-Barnes approximants for the renormalized vacuum polarization function. Although the estimated uncertainties from the omission of QED and isospin breaking in the gauge-field configurations, and from low-lying  $\pi\pi$  states in the vector-current correlators, are based on calculations for the leading-order vacuum polarization, they are about four times smaller, and do not contribute substantially to the total error. We obtain for the quark-connected contribution to  $a_\mu^{\text{HVP,HO}}$  with all systematics included

$$10^{10} a_\mu^{(\text{HO}, \text{conn.})} = -9.45(18)_{\text{lat.}} (55)_{\hat{\Pi}-\text{approx.}} (1.0)_{\log^2}, \quad (3.5)$$

where “lat.” denotes the sum of contributions associated with the underlying lattice-QCD calculations of the Taylor coefficients.

### C. Quark-disconnected contribution

Although several lattice-QCD calculations of the leading-order quark-disconnected contribution to  $a_\mu^{\text{HVP}}$  are available [7, 12, 44], these publications do not provide the Taylor coefficients of the renormalized vacuum polarization function.<sup>3</sup> We therefore estimate the values of the quark-disconnected Taylor coefficients assuming ground-state dominance of the vector-current correlators

<sup>3</sup> In Ref. [10], the BMW Collaboration provides the first two Taylor coefficients  $\Pi_1^{(\text{disc.})}$  and  $\Pi_2^{(\text{disc.})}$ , which are not sufficient to construct the [2,2] Padé and  $N = 2 + 1 + 1$  Mellin-Barnes approximants.

as in Ref. [44]. Using Eq. (11) of that work,

$$\frac{Q^2 \Pi_i^{(\text{disc.})}}{Q^2 \Pi_i^{(\text{conn.})}} = \frac{1}{10} \left[ \frac{m_\rho^{2j+2} f_\omega^2}{m_\omega^{2j+2} f_\rho^2} - 1 \right], \quad (3.6)$$

with  $\{M_\rho, M_\omega\} = \{0.77526(25), 0.78265(12)\}$  GeV from the PDG [45] and  $\{f_\rho, f_\omega\} = \{0.21(1), 0.20(1)\}$  GeV yields

$$Q^2 \Pi_1^{(\text{disc.})} / Q^2 \Pi_1^{(\text{conn.})} = -0.013(12), \quad (3.7)$$

and similar results for the higher Taylor coefficients. Both the leading  $O(\alpha^2)$  contribution to  $a_\mu^{\text{HVP}}$  and the dominant  $O(\alpha^3)$  contributions from diagrams (a) and (b) are proportional to the Taylor coefficient  $\Pi_1$  at lowest order in the small- $Q^2$  expansion. Further, the dominant quark-connected contribution is from the light up and down quarks. We therefore take  $-1.3(1.2)\%$  as the correction and uncertainty due to the omission of quark-disconnected contributions in our analysis. We note that our estimate in Eq (3.7) is consistent with recent lattice-QCD calculations of the leading-order quark-disconnected contribution with physical-mass pions from the BMW [12] and RBC/UKQCD Collaborations [7], who obtain for the ratio  $a_\mu^{(\text{LO,disc.})} / a_\mu^{(\text{LO,u/d conn.})}$  approximately  $-2.0\%$  and  $-1.5\%$ , respectively.

#### IV. RESULT AND OUTLOOK

We obtain the total  $O(\alpha_{\text{EM}}^3)$  hadronic vacuum polarization contribution to  $g_\mu - 2$  by adding our calculation of the quark-connected contribution, Eq. (3.5), to our estimate of the quark-disconnected contribution, Eq. (3.7). Our final result is

$$10^{10} a_\mu^{\text{HVP,HO}} = -9.3(0.6)_{\text{conn.}}(0.1)_{\text{disc.}}(1.0)_{\log^2}, \quad (4.1)$$

where the first two errors are from the quark-connected and quark-disconnected contributions, respectively. We list the error from omission of the “ $\log^2$ ” terms separately, since it does not arise from the use of lattice QCD to obtain the renormalized vacuum polarization function. This error could be eliminated with a different trick for expressing contribution (a) in terms of  $\hat{\Pi}(Q^2)$  than the one employed here. The uncertainty on the quark-connected contribution stems primarily from our use of Padé and Mellin-Barnes approximants for  $\hat{\Pi}(Q^2)$ , which we employ so that we can exploit already-published values of the Taylor coefficients. We anticipate reducing this error in a future paper that also includes an update of our determination of the leading-order hadronic vacuum polarization contribution [8] by calculating the higher-order contributions directly from the lattice correlation functions using the alternative formulae in Appendix A, and by analyzing a larger data set with more ensembles and finer lattice spacings.

Our result in Eq. (4.1) is the first lattice-QCD determination of the higher-order hadronic vacuum polarization

contribution to  $g_\mu - 2$ , and is consistent with determinations from  $e^+e^- \rightarrow \text{hadrons}$  data [14, 16, 21]. Although the lattice-QCD uncertainty is approximately ten times larger than from experiment plus dispersion relations, it is still below the target uncertainty of the Muon  $g - 2$  Experiment of 0.14 ppm, or  $\delta a_\mu \sim 1.6 \times 10^{-10}$  [3]. It therefore provides a new necessary ingredient in reaching the goal of obtaining a purely *ab-initio*-QCD determination of the hadronic contributions to  $g_\mu - 2$ .

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#### Appendix A: Formulae for higher-order HVP contributions to $g_\mu - 2$

Here we present integrals that can be used to calculate the higher-order hadronic-vacuum-polarization contributions to  $g_\mu - 2$  from lattice-QCD data. Our starting point is the expressions derived by Krause in Ref. [27] for the contributions from diagrams (a)–(c) in Fig. 2 in terms of  $R_\gamma(s)$  [Eq. (2.1)]. Contributions (b) and (c) can be expressed as the 1-loop QED integral for the lowest-order contribution from Blum [29] with a simple replacement of  $\hat{\Pi}(Q^2)$ , whereas contribution (a) is a nontrivial result of this work.

## 1. Contribution (a)

A complete analytical result for the contribution from the diagrams in (a) of Fig. 2 was first presented by Barbieri and Remiddi in Ref. [26]; in this work they also provide an expansion to first order in  $m_\mu^2/s$ . Later, in Ref. [27], Krause derived an asymptotic expansion for the kernel function in terms of the parameter  $r = m_\mu^2/s$ , which is more amenable to numerical integration. We start with the asymptotic expression given in Eq. (7) of Krause, which contains powers and logarithms of  $r$ .

Equation (7) does not have the form needed to exploit the relationship between  $R_\gamma(s)$  and the renormalized vacuum polarization function in Eq. (2.2). As suggested by Groote *et al.* [46], however, one can exploit generating integral representations of  $r^n$  and  $r^n \log(r)$  to express the pure polynomial and log terms in the asymptotic expansion of the kernel function in terms of  $\hat{\Pi}$ . Using Eqs. (39)–(42) of that work, and discarding terms proportional to  $\log^2(r)$  yields the following integral expression for contribution (a) in terms of the renormalized vacuum polariza-

tion function:

$$a_\mu^{(a)} = \left(\frac{\alpha}{\pi}\right)^3 \int_0^1 dx \left[ (a_0 + a_1 x + a_2 x^2 + a_3 x^3) \hat{\Pi}\left(\frac{m_\mu^2}{x}\right) + \frac{(b_0 + b_1 x + b_2 x^2 + b_3 x^3) \hat{\Pi}(m_\mu^2 x)}{x} \right], \quad (\text{A1})$$

with

$$\begin{aligned} a_0 &= -\frac{23}{18}, & b_0 &= \frac{61791297 - 7818200\pi^2}{1200}, \\ a_1 &= \frac{367}{108}, & b_1 &= -\frac{724746871}{1200} + \frac{152879\pi^2}{2}, \\ a_2 &= -\frac{10079}{1800}, & b_2 &= \frac{5364282053}{3600} - \frac{377219\pi^2}{2}, \\ a_3 &= \frac{6517}{900}, & b_3 &= -\frac{70906297}{72} + \frac{373975\pi^2}{3}. \end{aligned} \quad (\text{A2})$$

Checking the size of the omitted logarithmic terms using experimental data for  $R_\gamma(s)$  [31], we find that they are below  $1 \times 10^{-10}$ .

Alternatively, contribution (a) is given in terms of the Euclidean zero-momentum correlator by

$$a_\mu^{(a)} = \frac{4\alpha^3}{\pi} \int_0^\infty dt t^2 G(t) \tilde{K}_\ell^{(a)}(t), \quad (\text{A3})$$

with

$$\tilde{K}_\ell^{(a)}(t) = \frac{1}{t^2} \int_0^1 dx \left\{ \frac{1}{\omega^2} \sum_{i=0}^3 a_i x^i \left[ \omega^2 t^2 - 4 \sin^2\left(\frac{\omega t}{2}\right) \right] + \frac{1}{\omega'^2 x} \sum_{i=0}^3 b_i x^i \left[ \omega'^2 t^2 - 4 \sin^2\left(\frac{\omega' t}{2}\right) \right] \right\}, \quad (\text{A4})$$

and

$$\omega^2 = \frac{m_\mu^2}{x}, \quad \omega'^2 = m_\mu^2 x. \quad (\text{A5})$$

The factors of  $t^2$  and  $1/t^2$  in Eqs. (A3) and (A4), respectively, are chosen to make the kernel function  $\tilde{K}^{(a)}(t)$  dimensionless. With these formulae, contribution (a) can be obtained from a simple weighted sum of  $G(t)$  as in the leading-order case.

## 2. Contribution (b)

We start from Eq. (9) of Ref. [27] and make the change of variables  $Q^2 = m_\mu^2 x^2/(1-x)$ . The contribution from diagram (b) in Fig. 2 is then given in terms of the renormalized vacuum polarization function by

$$a_\mu^{(b)} = 8\pi^2 \left(\frac{\alpha}{\pi}\right)^3 \int_0^\infty dQ^2 K_E(Q^2) \hat{\Pi}(Q^2) F^\ell(m_e^2, Q^2), \quad (\text{A6})$$

where the lepton loop function is

$$F^\ell(m_e^2, x) = -\frac{8}{9} + \frac{\beta^3}{3} - \left(\frac{1}{2} - \frac{\beta^2}{6}\right) \beta \log\left(\frac{\beta-1}{\beta+1}\right), \quad (\text{A7})$$

$$\beta \equiv \sqrt{1 + 4\left(\frac{m_e^2}{Q^2}\right)}. \quad (\text{A8})$$

and  $K_E(Q^2)$  is the standard kernel function introduced by Blum in Ref. [29]:

$$K_E(Q^2) = \frac{1}{m_\mu^2} \cdot \hat{s} \cdot Z(\hat{s})^3 \cdot \frac{1 - \hat{s}Z(\hat{s})}{1 + \hat{s}Z(\hat{s})^2}, \quad (\text{A9})$$

$$Z(\hat{s}) = -\frac{\hat{s} - \sqrt{\hat{s}^2 + 4\hat{s}}}{2\hat{s}}, \quad \hat{s} = \frac{Q^2}{m_\mu^2}. \quad (\text{A10})$$

Thus, the expression in Eq. (A6) is simply the leading-order QED integral with the replacement  $\hat{\Pi}(Q^2) \rightarrow 8\pi\alpha \times \hat{\Pi}(Q^2) F^\ell(m_e^2, Q^2)$ . The analogous contribution from the  $\tau$  lepton is negligible because it is suppressed by  $m_\mu^2/m_\tau^2$ .



Contribution (b) can also be obtained from a weighted sum of the Euclidean zero-momentum correlator as in the

leading-order case:

$$a_\mu^{(b)}(m_\ell) = \frac{8\alpha^3}{\pi} \int_0^\infty dt t^2 G(t) \tilde{K}_\ell^{(b)}(t; m_\ell), \quad (\text{A11})$$

with the dimensionless kernel

$$\tilde{K}_\ell^{(b)}(t; m_\ell) = \frac{1}{t^2} \int_0^\infty d\omega \frac{4\pi^2 K_E(\omega^2)}{\omega^2} \left[ \omega^2 t^2 - 4 \sin^2 \left( \frac{\omega t}{2} \right) \right] F^\ell(m_\ell^2, \omega^2). \quad (\text{A12})$$

### 3. Contribution (c)

We start from Eq. (13) of Ref. [27]. Diagram (c) in Fig. 2 contains two hadronic insertions, and thus the contribution depends upon the square of the renormalized vacuum polarization function:

$$a_\mu^{(c)} = 4\pi^2 \left( \frac{\alpha}{\pi} \right)^3 \int_0^\infty dQ^2 K_E(Q^2) \hat{\Pi}(Q^2)^2. \quad (\text{A13})$$

In this case, the expression in Eq. (A13) has the form of the 1-loop QED integral, but with the replacement  $\hat{\Pi}(Q^2) \rightarrow 4\pi\alpha \times \hat{\Pi}(Q^2)^2$ .

When contribution (c) is expressed in terms of the Euclidean zero-momentum correlator, the two powers of the vacuum polarization function above yield two integrals over times  $t$  and  $t'$ :

$$a_\mu^{(c)} = 16\pi\alpha^3 \int_0^\infty dt t^2 G(t) \int_0^\infty dt' t'^2 G(t') \tilde{K}^{(c)}(t, t'), \quad (\text{A14})$$

with the dimensionless kernel

$$\tilde{K}^{(c)}(t, t') = \frac{1}{t^2 t'^2} \int_0^\infty d\omega \frac{4\pi^2 K_E(\omega^2)}{\omega^2} \left[ \omega^2 t^2 - \sin^2 \left( \frac{\omega t}{2} \right) \right] \left[ \omega^2 t'^2 - \sin^2 \left( \frac{\omega t'}{2} \right) \right]. \quad (\text{A15})$$

This formulation is slower to implement numerically than the analogous formulae for contributions (a) and (b) due to the double integral.

### Appendix B: Definition of $\hat{\Pi}_{2+1+1}(Q^2)$

In this paper we employ a slightly different form for the  $N = 2 + 1 + 1$  approximant for the Mellin transform of the hadronic spectral function than of the one given in Ref. [25], using

$$\mathcal{M}_{2+1+1}(s) = \frac{\alpha \sum_f Q_f^2}{3\pi} \left\{ \frac{1}{1-s} \frac{\Gamma(a-s)\Gamma(b-1)}{\Gamma(a-1)\Gamma(b-s)} + \frac{\Gamma(1-s)\Gamma(c-1)}{\Gamma(c-s)} + \frac{\Gamma(1-s)\Gamma(d-1)}{\Gamma(d-s)} \right\}, \quad (\text{B1})$$

with  $Q_f$  the charge of each quark flavor in units of  $e$ . We obtain the coefficients  $a$ - $d$  by solving the matching conditions

$$\mathcal{M}_{2+1+1}(-n) = \mathcal{M}_{\text{LQCD}}(-n), \quad n = \{0, 1, 2, 3\}, \quad (\text{B2})$$

where  $\mathcal{M}_{\text{LQCD}}(-n)$  are the lattice Mellin moments, and choosing the solution that satisfies  $\text{Re}(a, b, c, d) \geq 1$ ,

$\text{Im}(a, b) = 0$ , and  $c = d^*$ . The corresponding approximant for  $\hat{\Pi}(Q^2)$  is then given by the following sum of generalized hypergeometric functions:

$$\hat{\Pi}_{2+1+1}(Q^2) = \frac{\alpha \sum_f Q_f^2}{\pi} z \left\{ \frac{(a-1)}{(b-1)} {}_3F_2 \left[ \begin{matrix} 1 & 1 & a \\ & 2 & b \end{matrix}; -z \right] + \frac{1}{(c-1)} {}_2F_1 \left[ \begin{matrix} 1 & 1 \\ & c \end{matrix}; -z \right] + \frac{1}{(d-1)} {}_2F_1 \left[ \begin{matrix} 1 & 1 \\ & d \end{matrix}; -z \right] \right\}, \quad (\text{B3})$$

with

$$z = \frac{Q^2}{4m_\pi^2}. \quad (\text{B4})$$

### Appendix C: Quark-connected Taylor coefficients

Here we tabulate the values of the Taylor coefficients employed in our analysis. The light-quark connected  $\Pi_j$ s in Table IV include corrections for finite-volume and discretization effects as described in Ref. [8]. The charm- and bottom-quark connected  $\Pi_j$ s in Table V have already been extrapolated to the continuum in Refs. [22, 24].

TABLE IV. Light-quark-connected Taylor coefficients  $\Pi_j^{(ud)}$  and strange-quark-connected Taylor coefficients  $\Pi_j^{(s)}$  in units of  $1/\text{GeV}^{2j}$  [8, 23]. The quoted errors include statistics, the uncertainty on the vector-current renormalization factor, the (correlated) uncertainty from setting the lattice spacing, and the uncertainty on the corrections. The factor of the quarks' electromagnetic charges ( $Q_u^2 + Q_d^2$ ) is included in the definition of the  $\Pi_j$ s.

$\approx a$ (fm)	$\Pi_1^{(ud)}$	$\Pi_2^{(ud)}$	$\Pi_3^{(ud)}$	$\Pi_4^{(ud)}$	$\Pi_1^{(s)}$	$\Pi_2^{(s)}$	$\Pi_3^{(s)}$	$\Pi_4^{(s)}$
0.15	0.0889(12)	-0.1983(93)	0.728(69)	-4.05(55)	0.007387(83)	-0.00581(12)	0.00509(17)	-0.00453(20)
0.12	0.08704(97)	-0.1884(80)	0.682(62)	-3.82(49)	0.007361(82)	-0.00584(12)	0.00522(17)	-0.00477(21)

TABLE V. Charm- and bottom-quark-connected Taylor coefficients  $\Pi_j^{(f)}$  in units of  $1/\text{GeV}^{2j}$  [22, 24]. The quoted errors include statistics and all systematics. The factors of the quarks' electromagnetic charges  $Q_f^2$  are included in the definition of the  $\Pi_j$ s.

flavor	$10^3 \Pi_1^{(q)}$	$10^3 \Pi_2^{(q)}$	$10^3 \Pi_3^{(q)}$	$10^3 \Pi_4^{(q)}$
c	1.840(49)	-0.1240(43)	0.01081(43)	-1.030(41)e-3
b	0.0342(48)	-2.28(37)e-4	1.82(41)e-6	-1.57(49)e-8

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