Scale setting the Möbius Domain Wall Fermion on gradient-flowed HISQ action using the omega baryon mass and the gradient-flow scale \( w_0 \)

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We report on a sub-percent scale determination using the omega baryon mass and gradient-flow methods. The calculations are performed on 22 ensembles of \( N_f = 2+1+1 \) highly improved, rooted staggered sea-quark configurations generated by the MILC and CalLat Collaborations. The valence quark action used is Möbius Domain-Wall fermions solved on these configurations after a gradient-flow smearing is applied with a flowtime of \( t_{gf} = 1 \) in lattice units. The ensembles span four lattice spacings in the range \( 0.06 \lesssim a \lesssim 0.15 \) fm, six pion masses in the range \( 130 \lesssim m_\pi \lesssim 400 \) MeV and multiple lattice volumes. On each ensemble, the gradient-flow scale \( w_0/a \) and the omega baryon mass \( m_\Omega \) are computed. The dimensionless product of these quantities is then extrapolated to the continuum and infinite volume limits and interpolated to the physical light, strange and charm quark mass point in the isospin limit, resulting in the determination of \( w_0 = 0.1711(12) \) fm with all sources of statistical and systematic uncertainty accounted for. The dominant uncertainty in this result is the stochastic uncertainty, providing a clear path for a few-per-mille uncertainty, as recently obtained by the Budapest-Marseille-Wuppertal Collaboration.

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I. INTRODUCTION

Lattice QCD (LQCD) has become a prominent theoretical tool for calculations of hadronic quantities, and many calculations have reached a level of precision to
be able to supplement and/or complement experimental determinations [1]. Precision calculations of Standard Model processes, for example, are crucial input for experimental tests of fundamental symmetries in searches for new physics.

Lattice calculations receive only dimensionless bare parameters as input, so the output is inherently dimensionless. In some cases, dimensionless quantities or ratios of quantities may be directly computed without the need to determine any dimensional scale. Calculations of \( g_A \) and \( F_K/F_\pi \) are examples for which a precise scale setting is not necessary to make a precise, final prediction. However, there are many quantities for which a precise scale setting is desirable, such as the hadron spectrum, the nucleon axial radius, the hadronic contribution to the muon g − 2 [2] and many others.

In these cases, a quantity which is dimensionful (after multiplying or dividing by an appropriate power of the lattice spacing) is calculated and compared to experiment, following extrapolations to the physical point in lattice spacing, volume, and pion mass. Because the precision of any calculations of further dimensionful quantities is limited by the statistical and systematic uncertainties of this scale setting, quantities which have low stochastic noise and mild light quark mass dependence, such as the omega baryon mass \( m_\Omega \), are preferred. The lattice spacing on each ensemble may then be determined by comparing the quantity calculated on a given ensemble to the continuum value.

However, the most precise quantities one may calculate are not necessarily accessible experimentally. For example, the Sommer scale \( r_0 \) [3] has been one of the most commonly used scales. This scale requires a determination of the heavy-quark potential which is susceptible to fitting systematic uncertainties. More recently, the gradient flow scale \( w_0 \) [4] has been used recently for a more precise determination of the lattice spacing [5–12]. In this case, a well-controlled extrapolation of this quantity to the physical point is also necessary.

In this paper we present a precision scale setting for our mixed lattice action [13] which uses \( N_f = 2 + 1 + 1 \) highly improved, rooted staggered sea-quark (HISQ) configurations generated by the MILC [14] and CalLat Collaborations and Möbius Domain-Wall fermions for the valence sector. We compute the dimensionless product \( m_\Omega w_0 \) on each ensemble and extrapolate to the physical point, giving us a determination for \( w_0 \) with all systematics accounted for,

\[
\begin{align*}
w_0 m_\Omega &= 1.450(8)^s(5)^\chi(03)^a(00)^V(00)^{\text{phys}}(02)^M \\
&= 1.450(10) \\
\frac{w_0}{m_\Omega} &= 0.1711(09)^s(06)^\chi(03)^a(00)^V(00)^{\text{phys}}(02)^M \\
&= 0.1711(12) ,
\end{align*}
\]

with the statistical (s), chiral (\( \chi \)), continuum-limit (a), infinite volume (V), physical-point (phys), and model selection uncertainties (M).

We then perform an interpolation of the values of \( w_0/a \) to the infinite volume and physical quark mass limits which allows us to provide a precise, quark mass independent scale setting for each lattice spacing, with our final results in Eq. (4.10). In the following Sections we provide details of our lattice setup, our methods for extrapolation, and our results with uncertainty breakdown. We conclude with a discussion in the final Section.

II. DETAILS OF THE LATTICE CALCULATION

A. MDWF on gradient-flowed HISQ

The lattice action we use is the mixed-action [18, 19] with Möbius [20] Domain-Wall Fermions [21–23] solved on \( N_f = 2 + 1 + 1 \) highly improved staggered quarks [24] after they are gradient-flow smeared [25–27] (corresponding to an infinitesimal stout-smearing procedure [28]) to a flow-time of \( t_{\text{sf}}/a^2 = 1 \) [13]. The choice to hold the flow-time fixed in lattice units is important to ensure that as the continuum limit is taken, effects arising from finite flow-time also extrapolate to zero.

This action has been used to compute the nucleon axial coupling, \( g_A \), with a 1% total uncertainty [29–32], the \( \pi^- \to \pi^+ \) matrix elements relevant to neutrinoless double beta-decay [33] and most recently, \( F_K/F_\pi \) [34]. Our calculation of \( F_K/F_\pi \) was obtained with a total uncertainty of 0.4% which provides an important benchmark for our action, as the result is consistent with other determinations in the literature [7, 10, 35–42] (and the FLAG average [1]), and also contributes to the test of the universality of lattice QCD results in the continuum limit.

Our plan to compute the axial and other elastic form factors of the nucleon with this mixed-action, as well as other quantities, leads to a desire to have a scale setting with sufficiently small uncertainty that it does not increase the final uncertainty of such quantities. It has been previously observed that both \( w_0 \) [4, 11] and the omega baryon mass [12, 43–49] have mild quark mass dependence and that they can be determined with high statistical precision with relatively low computational cost. The input parameters of our action on all ensembles are provided in Table I.

B. Correlation function construction and analysis

For the scale setting computation, we have to determine four or five quantities on each ensemble, the pion, kaon and omega masses, the gradient-flow scale \( w_0 \) and the pion decay constant \( F_\pi \). For \( m_\pi, m_K \) and \( F_\pi \), we take the values from our \( F_K/F_\pi \) computation for the 18 ensembles in common. For the four new ensembles in this work (a15m310L, a12m310XL, a12m220ms, a12m180L), we follow the same analysis strategy described in Ref. [34].
| ensemble     | \( \beta \) | \( N_{cutoff} \) | volume | \( a_{\text{min}} \) | \( a_{\text{max}} \) | \( L_2/a \) | \( aM_{S} \) | \( b_{0,c} \) | \( aM_{\pi} \) | \( aM_{\pi}^{\text{inv}} \times 10^{4} \) | \( aM_{\pi}^{\text{val}} \) | \( aM_{\pi}^{\text{val}}^{\text{inv}} \times 10^{4} \) | \( \sigma \) | \( N_{\text{src}} \) |
|-------------|-----------|----------------|--------|----------------|----------------|---------|----------|--------|----------|----------------------------|-------------|----------------------------|----------|--------|
| a15m400\(^a\) | 5.80      | 1000 \( \times 48 \) | 0.0217 | 0.065          | 0.838          | 12.1.3  | 1.50     | 0.50    | 0.0278  | 9.365(67)                               | 0.0902      | 6.937(63)                               | 3.0      | 30     |
| a15m350\(^a\) | 5.80      | 1000 \( \times 48 \) | 0.0166 | 0.065          | 0.838          | 12.1.3  | 1.50     | 0.50    | 0.0206  | 9.416(90)                               | 0.0902      | 6.688(62)                               | 3.0      | 30     |
| a15m310\(^a\) | 5.80      | 1000 \( \times 48 \) | 0.013  | 0.065          | 0.838          | 12.1.3  | 1.50     | 0.50    | 0.0158  | 9.563(67)                               | 0.0902      | 6.640(44)                               | 4.2      | 45     |
| a15m310L\(^a\) | 5.80     | 1000 \( \times 48 \) | 0.013  | 0.065          | 0.838          | 12.1.3  | 1.50     | 0.50    | 0.0158  | 9.581(50)                               | 0.0902      | 6.581(37)                               | 4.2      | 45     |
| a15m220     | 5.80      | 1000 \( \times 48 \) | 0.0064 | 0.064          | 0.828          | 16.1.3  | 1.75     | 0.75    | 0.0072  | 7.536(38)                               | 0.0902      | 3.890(25)                               | 4.5      | 60     |
| a15m135XL\(^a\) | 5.80     | 1000 \( \times 48 \) | 0.004246 | 0.06730     | 0.8447         | 24.1.3 | 2.25     | 1.25    | 0.00237 | 2.706(08)                               | 0.0945      | 1.860(09)                               | 3.0      | 30     |
| a12m400\(^a\) | 6.00      | 1000 \( \times 48 \) | 0.0170 | 0.0599        | 0.635          | 8.1.2   | 1.25     | 0.25    | 0.0219  | 7.337(50)                               | 0.0903      | 5.129(35)                               | 3.0      | 30     |
| a12m350\(^a\) | 6.00      | 1000 \( \times 48 \) | 0.0130 | 0.0599        | 0.635          | 8.1.2   | 1.25     | 0.25    | 0.0166  | 7.579(52)                               | 0.0903      | 5.062(34)                               | 3.0      | 30     |
| a12m310\(^a\) | 6.00      | 1005 \( \times 48 \) | 0.0102 | 0.0599        | 0.635          | 8.1.2   | 1.25     | 0.25    | 0.0126  | 7.702(52)                               | 0.0903      | 4.950(35)                               | 3.0      | 30     |
| a12m310XL\(^a\) | 6.00    | 1000 \( \times 48 \) | 0.0102 | 0.0599        | 0.635          | 8.1.2   | 1.25     | 0.25    | 0.0126  | 7.728(22)                               | 0.0903      | 4.927(21)                               | 3.0      | 30     |
| a12m220S     | 6.00      | 1000 \( \times 48 \) | 0.00507 | 0.0507     | 0.628          | 12.1.2  | 1.50     | 0.50    | 0.00600 | 3.990(42)                               | 0.0903      | 2.390(24)                               | 6.0      | 90     |
| a12m220ms    | 6.00      | 1000 \( \times 48 \) | 0.00507 | 0.0507     | 0.628          | 12.1.2  | 1.50     | 0.50    | 0.00600 | 4.050(20)                               | 0.0903      | 2.364(15)                               | 6.0      | 90     |
| a12m220ms    | 6.00      | 1000 \( \times 48 \) | 0.00507 | 0.0507     | 0.628          | 12.1.2  | 1.50     | 0.50    | 0.00600 | 3.819(26)                               | 0.0903      | 2.364(15)                               | 6.0      | 90     |
| a12m220ms    | 6.00      | 1000 \( \times 48 \) | 0.00507 | 0.0507     | 0.628          | 12.1.2  | 1.50     | 0.50    | 0.00600 | 4.040(26)                               | 0.0903      | 2.361(19)                               | 6.0      | 90     |

\(^a\) Additional ensembles generated by CalLat using the MILC code. The m350 and m400 ensembles were made on the Vulcan supercomputer at LLNL while the a12m310XL, a15m180L, a15m310XL, a09m135, and a06m310L ensembles were made on the Sierra and Lassen supercomputers at LLNL and the Summit supercomputer at OLCF using QUDA [16, 17]. These configurations are available to any interested party upon request, and will be available for easy anonymous downloading—hopefully soon.

The a12m220ms ensemble is identical to a12m220 except that the strange quark mass is roughly 60% of the physical value rather than being near the physical value. The a15m310L ensemble has identical input parameters as the a15m310 ensemble but \( L = 24 \) (3.6 fm) instead of \( L = 16 \) (2.4 fm), while the a12m310XL ensemble is identical to the a12m310 ensemble but with \( L = 48 \) (5.8 fm) instead of \( L = 24 \) (2.9 fm). The a12m180L and a12m310XL ensembles have a lattice volume that is the same size as a12m130 but pion masses of roughly \( m_{\pi} \approx 180 \) and 310 MeV. These new ensembles provide important lever arms for the various extrapolations. The a12m220ms provides a unique lever arm for varying the strange quark mass significantly from its physical value, the a15m310L and a12m310XL provide other pion masses where we can perform a volume study and the a12m180L ensemble provides an additional light pion mass ensemble to help with the physical pion mass extrapolation. The first of these is important for this scale setting while the latter three will be more important for future work.

The omega baryon correlation functions are constructed similarly to the pion and kaon. A source for the propagator is constructed with the gauge invariant Gaussian smearing routine in Chroma [50]. \textsc{(Gauge	extunderscore Inv	extunderscore Gaussian)}. Then, correlation functions are constructed using both a point sink as well as the same gauge invariant Gaussian smearing routine with the same parameters as the source. The values of the “smearing width” (\( \sigma \)) and the number of iterations (\( N \)) used to approximate the exponential smearing profile are provided in Table I. The correlation functions constructed with the point sink are referred to as PS and those with the smeared sink as SS.

Local spin wave-functions are constructed following Refs. [51, 52]. Both positive- and negative-parity omega-baryon correlation functions are constructed with the upper and lower spin components of the quark propagators in the Dirac basis. The negative-parity correlation functions are time-reversed with an appropriate sign flip of the correlation function, effectively doubling the statistics with no extra inversions. The four different spin projections of the omega are averaged as well to produce the final spin and parity averaged two-point correlation functions.

The reader will notice that the values of \( \sigma \) and \( N \) do not follow an obvious pattern. This is because in our first extraction of the ground state and did not show signs of large negative overlap factors. Hence, many but not
FIG. 1. Stability plots of the ground state omega baryon mass on the three physical pion mass ensembles. The left plots show the effective mass data (in lattice units) and reconstructed effective mass from the chosen fit for both the SS and PS correlation functions. The dark gray and colored band are displayed for the region of time used in the analysis and an extrapolation beyond \( t_{\text{max}} \) is shown after a short break in the fit band. The horizontal gray band is the prior used for the ground state mass. The right plots show the corresponding value of \( E_0 \) as a function of \( t_{\text{min}} \) and the number of states \( n_s \) used in the analysis, as well as the corresponding \( Q \) value and relative weight as a function of \( n_s \) for a given \( t_{\text{min}} \), where the weight is set by the Bayes Factor. See App. A for more detail on the selection of the final fit. The chosen fit is denoted with a filled black symbol and the horizontal band is the value of \( E_0 \) from the chosen fit. The \( y \)-range of the upper panel of the stability plots is equal to the prior of the ground state energy (the horizontal gray band in the left plot).

all of the ensembles have been rerun with our improved choices of \( \sigma \) and \( N \). We have observed the choice \( \sigma = 3.0 \) and \( N = 30 \) works well for the a15 and a12 ensembles and that \( \sigma = 3.5 \) with \( N = 45 \) works well for the a09 and a06 ensembles.

In order to determine the omega baryon mass on each ensemble, we perform a stability analysis of the extracted ground state mass as a function of \( t_{\text{min}} \) used in the fit as well as the number of states used in the analysis. The correlation functions are analyzed in a Bayesian framework with constraints [55]. We choose normally distributed priors for the ground-state energy and all overlap fac-
tors, and log-normal distributions for excited-state energy priors. The ground-state energy and overlap factors are motivated by the plateau values of the effective masses with the priors taken to be roughly 10 times larger than the stochastic uncertainty of the respective effective mass data in the plateau region. The excited-state energy splittings are set to the value of two pion masses with a width allowing for fluctuations down to one pion mass within one standard deviation.

In Fig. 1 we show sample extractions of the ground state mass on our three physical pion mass ensembles. In the left plot, we show the effective mass data from the two correlation functions. The weights are normalized on a given time slice by the largest Bayes factor at that \( t_{\text{min}} \) value. We have not implemented a more thorough algorithm to weight fits against each other that utilize different amounts of data, as described for example in Ref. [56]. Rather, we have chosen a fit for a given ensemble (the filled black symbol in the right panels highlighted by the horizontal colored band) that has a good fit quality, the maximum or near maximum relative weight, and consistency with the late-time data. We tried to optimize this choice over all ensembles simultaneously, with \( t_{\text{min}} \) held nearly fixed for a given lattice spacing, rather than hand-picking the optimal fit on each ensemble separately, in order to minimize the possible bias introduced by analysis choices. Good fits are obtained on all ensembles with \( n_s = 2 \), simplifying the model function and reducing the chance of overfitting the correlation functions, which is most relevant on ensembles with the more aggressive choices of smearing parameters. In App. C, we show the corresponding stability plots for all remaining ensembles. In Table II we show the resulting values of \( am_\Omega \) on all ensembles used in this work.

C. Calculation of \( w_0 \)

In order to efficiently compute the value of \( w_0/a \) on each ensemble, we have implemented the Symanzik flow in the QUDA library [16, 17, 57]. We used the tree-level improved action and the symmetric, cloverleaf definition of the field-strength tensor, following the MILC implementation [58]. We used a step size of \( \epsilon = 0.01 \) in the Runge-Kutta algorithm proposed by Lüscher [59], which leads to negligibly small integration errors. In Fig. 2, we show the determination of the flow-time on the two new physical pion mass ensembles we have generated, defined by the point [4]

\[
W \equiv \left. \frac{d}{dt} (t^2 \langle E(t) \rangle) \right|_{t = w_0^2} = 0.3, \tag{2.1}
\]

where \( \langle E(t) \rangle \) is the gluonic action density at flow time \( t \). The values of \( w_0/a \) as well as the correlated product \( w_0 m_\Omega \) are provided in Table II for all ensembles. The uncertainties are determined by observing a saturation of the uncertainty as the bin-size is increased when binning the results from configurations close in Monte Carlo time. These uncertainties were cross-checked with an autocorrelation study using the \( \Gamma \)-method [60] implemented in the \texttt{new} Python package [61].

III. EXTRAPOLATION FUNCTIONS

This work utilizes 22 different ensembles, each with O(1000) configurations (Table I), to control the systematic uncertainties in the LQCD calculation of the scale. This allows us to address:

1. The physical light and strange quark mass limit;
2. The physical charm quark mass limit;
3. The continuum limit;
4. The infinite volume limit.

1. Physical light and strange quark mass limit

The ensembles have a range of light quark masses which correspond roughly to \( 130 \lesssim m_\pi \lesssim 400 \) MeV. We have three lattice spacings at \( m_\pi \simeq m_\pi^{\text{phys}} \) such that the light quark mass extrapolation is really an interpolation. On all but one of the 22 ensembles, the strange quark
mass is close to its physical value, allowing us to perform a simple interpolation to the physical strange quark mass point. One ensemble has a strange quark mass of roughly 2/3 its physical value (a12m220ms), allowing us to explore systematics in this strange quark mass interpolation.

To parameterize the light and strange quark mass dependence, we utilize two sets of small parameters:

\begin{align}
\Lambda &= F : \quad l_F^2 = \frac{m_F^2}{\Lambda^2}, \quad s_F^2 = \frac{2m_K^2 - m_F^2}{\Lambda^2}, \\
\Lambda &= \Omega : \quad l_\Omega^2 = \frac{m_\Omega^2}{m_\Omega^2}, \quad s_\Omega^2 = \frac{2m_K^2 - m_\Omega^2}{m_\Omega^2},
\end{align}

where we have defined

\[ \Lambda_\chi = 4\pi F_\chi. \]

Using the Gell-Mann–Oakes–Renner relation [62], the numerators in these parameters correspond roughly to the light and strange quark mass, \[ m_F^2 = 2B\bar{m}\] and \[ 2m_K^2 - m_F^2 = 2Bm_s, \]
where \( \bar{m} = \frac{1}{2}(m_u + m_d) \). The first set of parameters, Eq. (3.1), is inspired by \( yPT \) and commonly used as a set of small expansion parameters in extrapolating LQCD results. The second set of small parameters, Eq. (3.2), is inspired by Ref. [45]. In Fig. 3, we plot the values of these parameters in comparison with the physical point. Since we are working in the isospin limit in this work, we define the physical point as

\[ \begin{align*}
  m_{\pi}^{\text{phys}} &= 134.8(3) \text{ MeV}, \\
  m_{K}^{\text{phys}} &= \tilde{M}_{K} = 494.2(3) \text{ MeV}, \\
  F_{\pi}^{\text{phys}} &= F_{\pi^{\text{phys}}} = 92.07(57) \text{ MeV}, \\
  m_{\Omega}^{\text{phys}} &= 1672.43(32) \text{ MeV},
\end{align*} \]

with the first three values from the FLAG report [1] and the omega baryon mass from the PDG [63]. The values of \( l_{F,\Omega} \) and \( s_{F,\Omega} \) are given in Table II for all ensembles.

2. Physical charm quark mass limit

The FNAL and MILC collaborations have provided a determination of the input value of the charm quark mass that reproduces the “physical” charm quark mass for each of the four lattice spacings used in this work. The mass of the \( D_s \) meson was used to tune the input charm quark mass until the physical \( D_s \) mass was reproduced (with the already tuned values of the input strange quark mass), defining the “physical” charm quark masses [39],

\[ \begin{align*}
  a_{15} m_{c}^{\text{phys}} &= 0.8447(15), \quad a_{12} m_{c}^{\text{phys}} = 0.6328(8), \\
  a_{09} m_{c}^{\text{phys}} &= 0.4313(6), \quad a_{06} m_{c}^{\text{phys}} = 0.2579(4).
\end{align*} \]

Comparing to Table I, the simulated charm quark mass is mistuned by less than 2% of the physical charm quark mass.
mass for all ensembles used in this work except the $a06m310L$ ensemble, whose simulated charm quark mass is almost 10% heavier than its physical value.

In order to test the sensitivity of our results to this mistuning of the charm quark mass, we perform a reweighting study of the $a06m310L$ correlation functions and extracted pion, kaon and omega baryon masses. While not sensitive to this mistuning of the charm quark mass, we find that the splitting is determined under bootstrap. We in line with prior expectation. For example, we find

$$\delta a_{06} m_c = a_{06} m_c^{\text{phys}} - a_{06} m_c^{\text{HMC}} = -0.0281(4).$$

(3.6)

As the reweighting factor is provided by a ratio of the charm quark fermion determinant, it is an extensive quantity, and the relatively large volume we have used to generate the $a06m310L$ ensemble causes some challenges in accurately determining the reweighting factor.

The summary of our study is that our scale setting is in Fig. 4. The small dimensionless parameter we utilize in this work expressed in terms of $l_F^2$ and $\epsilon_a^2$.

to extrapolate to the continuum limit is

$$\epsilon_a = \frac{a}{2w_0}. \quad (3.8)$$

As noted in Ref. [34], this choice is convenient as the values of $\epsilon_a^2$ span a similar range as $l_F^2$. This allows us to test the ansatz of our assumed power counting that treats corrections of $O(l_F^2) = O(\epsilon_a^2)$ which we found to be the case for $F_K/F_\pi$ [34].

4. Infinite volume limit

The leading sensitivity of $m_\Omega$ and $w_0$ to the size of the volume is exponentially suppressed for sufficiently large $m_\pi L$ [65]. We have ensembles with multiple volumes at $a15m310$, $a12m310$ and $a12m220$ to test the predicted finite volume corrections against the observed ones. We derive the predicted volume dependence of $w_0m_\Omega$ to the first two non-trivial orders in Sec. III B.

We now turn to the derivation of the extrapolation formula for each of these systematic uncertainties.
A. Light and Strange Quark Mass Dependence

The light and strange quark mass dependence of the omega baryon has been derived in $SU(3)$ heavy baryon CHPT [66, 67] to next-to-next-to-leading order (N^3LO) which is O($m_{\Omega,K}^6$) [68–70]. It has been shown that $SU(3)\ HB\ CHPT$ does not produce a converging expansion at the physical quark masses [44, 71–74], and so using these formulas to obtain a precise, let alone subpercent, determination, at the physical pion mass is not possible when incorporating systematic uncertainties associated with the truncation of $SU(3)\ HB\ CHPT$.

However, many LQCD calculations, including this one, keep the strange quark mass fixed near its physical value. Therefore, a simple interpolation in the strange quark mass is possible. Further, as the omega is an isosinglet, it will have a simpler, and likely more rapidly converging chiral expansion of the light-quark mass dependence than baryons with one or more light valence quarks. This has motivated the construction of an $SU(2)$ HB CHPT for hyperons which considers only the pion as a light degree of freedom [75–79]. In particular, the chiral expansion for the omega baryon mass was determined to O($m_{\Omega}^{6}$) [76]

$$m_{\Omega} = m_0 + \alpha_2 \frac{m_{\pi}^2}{\Lambda^2} + m_{\pi}^4 \left( \alpha_4 \lambda_{\pi} + \beta_4 \right)$$

$$+ \frac{m_0^6}{\Lambda^6} \left[ \alpha_6 \lambda_{\pi}^2 + \beta_6 \lambda_{\pi} + \gamma_6 \right],$$  \hspace{1cm} (3.9)

where

$$\lambda_{\pi} = \lambda_{\pi}(\mu) = \ln \left( \frac{m_{\pi}^2}{\mu^2} \right)$$  \hspace{1cm} (3.10)

$\alpha_n$, $\beta_n$ and $\gamma_6$ are linear combinations of $\mu$-dependent dimensionless low energy constants (LECs) of the theory, and $m_0$ is the mass of the omega baryon in the $SU(2)$ chiral limit at the physical strange quark mass. The renormalization group [80] restricts the coefficient of the $\ln^2$ term to be linearly dependent on $\alpha_2$ and $\alpha_4$, with the relation provided in Ref. [76]. In standard HB CHPT power counting, in which the expansion includes odd powers of the pion mass, this order would be called next-to-next-to-next-to-leading order (N^3LO), where leading order (LO) is the O($m_{\Omega}^2/\Lambda^2$) contribution, next-to-leading order (NLO) would be an O($m_{\Omega}^4/\Lambda^2$) contribution, which vanishes for $m_{\Omega}$, etc.

The light quark mass dependence for $w_0$ has also been determined in $\chi$PT through O($m_{\pi}^2$) [81] which is N^2LO in the meson chiral power counting

$$w_0 = w_{0,\text{ch}} \left\{ 1 + k_1 \frac{m_{\pi}^2}{\Lambda^2} + k_3 \frac{m_{\pi}^4}{\Lambda^4} + k_2 \frac{m_{\pi}^4 \lambda_{\pi}}{\Lambda^4} \right\},$$  \hspace{1cm} (3.11)

where the LO term, $w_{0,\text{ch}}$, is the value in the chiral limit and the $k_i$ are linear combinations of dimensionless LECs.

From these expressions, we can see both $m_{\Omega}$ and $w_0$ depend only upon even powers of the pion mass through the order we are working: $m_{\Omega}$ receives a chiral correction that scales as O($m_{\pi}^2$) from a double-sunset two-loop diagram [76] and the next correction to $w_0$ will appear at O($m_{\pi}^6$). We may multiply these expressions together, Eq. (3.9) and (3.11), in order to form an expression describing the light-quark mass dependence of $w_0m_{\Omega}$. As the characterization of the order of the expansion with respect to the order of $m_{\pi}^2$ is not the same for $w_0$ and $m_{\Omega}$, we define the contributions to $w_0m_{\Omega}$ as

$$w_0m_{\Omega} = c_0 + \delta_{l,s}^{\text{NLO}} + \delta_{l,s}^{\text{N^2LO}} + \delta_{l,s}^{\text{N^3LO}}.$$  \hspace{1cm} (3.12)

We add polynomial terms in $s_{l,s}^2$ such that

$$\delta_{l,s}^{\text{NLO}} = \frac{\Lambda}{\pi} c_1 + s_{l,s}^2 c_s,$$

$$\delta_{l,s}^{\text{N^2LO}} = \frac{\Lambda}{\pi} (c_{l} + c_{l}^{\text{NLO}}) + s_{l,s}^2 c_{l,s} + s_{l,s}^4 c_{s,s},$$

$$\delta_{l,s}^{\text{N^3LO}} = \frac{\Lambda}{\pi} (c_{l} + c_{l}^{\text{NLO}}) + c_{l}^{\text{N^2LO}} c_{l,s} + s_{l,s}^2 \frac{\Lambda}{\pi} c_{l,s} + s_{l,s}^4 c_{s,s}$$

$$+ \frac{\Lambda}{\pi} s_{l,s}^2 c_{l,s} + s_{l,s}^4 c_{l,s} + s_{l,s}^6 c_{s,s}.$$  \hspace{1cm} (3.13)

We will consider both $\Lambda = F$ and $\Lambda = \Omega$ for the two choices of small parameters. For convenience, we set $\mu = \Lambda$ and $\mu = m_{\Omega}$ respectively for these choices. For a detailed discussion how one can track the consequence of such a quark mass dependent choice for the dim-reg scale, see Ref. [34].

B. Finite Volume Corrections

The finite-volume (FV) corrections for $m_{\Omega}$ are determined at one loop through the modification to the tadpole integral [82, 83]

$$\frac{(4\pi)^2}{m^2} F^{\text{FV}} = \ln \left( \frac{m_{\pi}^2}{\mu^2} \right) + 4k_1(m_{\pi}L)$$  \hspace{1cm} (3.14)

where $k_1(x)$ is given by

$$k_1(x) = \sum_{|\mathbf{n}| \neq 0} c_n \frac{K_1(x|\mathbf{n})}{x|\mathbf{n}|}.$$  \hspace{1cm} (3.15)

$K_1(x)$ is a modified Bessel function of the second kind and $c_n$ are multiplicity factors for the number of ways the integers ($n_x, n_y, n_z$) can form a vector of length $|\mathbf{n}|$, see Table III for the first few.

At N^3LO, the finite volume corrections for $m_{\Omega}$ are also trivially determined, as the only two-loop integral that contributes is a double-tadpole with un-nested momentum integrals, see Fig. 2 of Ref. [76]. The N^3LO correction to $w_0$ is not known. However, the isoscalar nature

| $|\mathbf{n}|$ | 1 | $\sqrt{2}$ | $\sqrt{3}$ | $\sqrt{4}$ | $\sqrt{5}$ | $\sqrt{6}$ | $\sqrt{7}$ | $\sqrt{8}$ | $\sqrt{9}$ | $\sqrt{10}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| $c_n$ | 6 | 12 | 8 | 6 | 24 | 24 | 0 | 12 | 30 | 24 |
of \( w_0 \) means that at the two-loop order, just like the correction to \( m_\Omega \), it will only receive contributions from trivial two-loop integrals with factorizable momentum integrals. Therefore, the \( N^3 \) LO FV correction can also be determined from the square of the tadpole integral

\[
\frac{(4\pi)^4}{m^4} \left[ (I^{\text{FV}})^2 - (I^{\infty})^2 \right] = 8\lambda_\pi k_1(m_\pi L) + 16k_1^2(m_\pi L) ,
\]
resulting in

\[
\delta_{L,F}^{N^3 \text{LO}}(l_F, m_\pi L) = c_{ll}^{\eta 4} l_F^4 k_1(m_\pi L)
\]

\[
\delta_{L,F}^{N^3 \text{LO}}(l_F, m_\pi L) = c_{ll}^{\eta 2} l_F^2 \ln(l_F) 8k_1(m_\pi L) + c_{ll}^{\eta 2} l_F^2 16k_1(m_\pi L).
\]

The FV correction through \( N^3 \) LO arising from loop corrections to \( w_0 \) and \( m_O \) is given by

\[
\delta_{L,F} = \delta_{L,F}^{N^2 \text{LO}} + \delta_{L,F}^{N^3 \text{LO}},
\]
with a similar expression for \( \delta_{L,\Omega} \).

We are neglecting a few FV corrections at \( \delta_{L,F}^{N^3 \text{LO}} \). The NLO \( l_F^2 \Omega \) correction to the omega mass is from a quark mass operator, which has been converted to an \( m_\pi \) correction, \( 2B_\Omega m_\pi = m_\pi^2 + O(m_\pi^3 / \Lambda^3) \). This choice for organizing the perturbative expansion induces corrections in what we have called \( N^3 \) LO and \( N^3 \) LO. At \( N^3 \) LO, the corrections arise from single tadpole diagrams and so the FV corrections are accounted for through Eq. (3.17). At the next order, the corrections to the pion self-energy involve more complicated two-loop diagrams \([84]\) and so the FV corrections arising from these are not captured in our parametrization. Similar corrections arise from expressing \( 4\pi F_0 = 4\pi F_\pi + O(m_\pi^2 / \Lambda^2) \) when using \( l_F^2 \) to track the light-quark mass corrections \( F_0 \) is \( F_\pi \) in the \( SU(2) \) chiral limit.

While we have neglected these contributions, the FV corrections to \( m_\Omega \) are suppressed by an extra power in the chiral power counting compared with many observables, beginning with an \( m_\pi^2 / \Lambda^2 \) prefactor, Eq. (3.17). In Fig. 5, we show the predicted FV correction along with the results at three volumes on the \( a12 \ m_2 / 20 \) ensembles. As can be observed, the predicted FV corrections are very small and consistent with the numerical results.

C. Discretization Corrections

A standard method of incorporating discretization effects into the extrapolation formula used for hadronic observables is to follow the strategy of Sharpe and Singleton \([85]\):

1. For a given lattice action, one first constructs the Symanzik Effective Theory (SET) by expanding the discretized action about the continuum limit. This results in a local effective action in terms of quark and gluon fields \([85, 87]\);

2. With this continuum effective theory, one builds a chiral effective theory by using spurion analysis to construct not only operators with explicit quark mass dependence, but also operators with explicit lattice spacing dependence.

Such an approach captures the leading discretization effects in a local hadronic effective theory. At the level of the SET, radiative corrections generate logarithmic dependence upon the lattice spacing. The leading corrections can be resummed such that, for an \( O(a) \) improved action, the leading discretization effects then scale as \( a^2 \alpha_s^{n+\gamma_1} \) \([88, 89]\) where \( n = 0 \) for an otherwise unimproved action, \( n = 1 \) for a perturbatively improved action and \( n = 2 \) for a non-perturbatively improved action. The coefficient \( \gamma_1 \) is an anomalous dimension which has been determined for Yang-Mills and Wilson actions \([90]\).

For mixed-action setups \([18, 19]\) such as the one used in this work, a low-energy mixed-action Effective Field Theory (MAEFT) \([19, 91–99]\) can be constructed to capture the manifestation of infrared radiative corrections from the discretization\(^1\). Corrections come predominantly from a modification of the pseudoscalar meson spectrum as well as from “hairpin” interactions \([100]\) that are proportional to the lattice spacing in rooted-staggered \([101]\) and mixed-action theories \([93]\); in partially-quenched theories, these hairpins are proportional to the difference in the valence and sea quark masses \([102–104]\).

In our analysis of \( F_K / F_\pi \), we observed that the use of continuum chiral perturbation theory with corrections polynomial in \( c_\pi^2 \) was highly favored over the use of the MAEFT expression, as measured by the Bayes-Factor,

\(^1\) While this might seem counterintuitive, it is analogous to the infrared sensitivity of hadronic quantities to the Higgs vacuum expectation value (vev): hadronic quantities have infrared (logarithmic) sensitivity to the pion mass from radiative pion loops, and the squared pion mass is proportional to the light quark mass which is proportional to the Higgs vev.
though the results from both were consistent within a fraction of one standard deviation [34]. Similar findings have been observed by other groups for various quantities, see for example Refs. [105–107]. Therefore, in this work, we restrict our analysis to a continuum-like expression enhanced by polynomial discretization terms.

The dynamical HISQ ensembles have a perturbatively improved action such that the leading discretization effects (before resumming the radiative corrections [88–90]) scale as $O(\alpha_s a^2)$ [24]. The MDWF action, in the limit of infinite extent in the fifth dimension, has no chiral symmetry breaking other than that from the quark mass. Consequently, the leading discretization corrections begin at $O(a^2)$ [108, 109]. For finite $L_5$, the $O(a)$ corrections are proportional to $a m_{\text{res}}$ which is sufficiently small that these terms are numerically negligible. Therefore, we parametrize our discretization corrections with the following terms where we count $\epsilon_a^2 \sim l_F^2 \sim s_\Lambda^2$

$$
\delta_{a,\Lambda} = \delta_{a,\Lambda}^{\text{NLO}} + \delta_{a,\Lambda}^{N^2\text{LO}} + \delta_{a,\Lambda}^{\text{NLO}} ,
$$

$$
\delta_{a,\Lambda}^{\text{NLO}} = d_a s_a^2 + d'_a a S_a^2 ,
$$

$$
\delta_{a,\Lambda}^{N^2\text{LO}} = d_{aa} a^2 + c^2 (d_{aal} l_F^2 + d_{ass}s_\Lambda^2) ,
$$

$$
\delta_{a,\Lambda}^{\text{NLO}} = d_{aaa} a^6 + c^4 (d_{aal} l_F^2 + d_{ass}s_\Lambda^2) + c^6 (d_{aal} l_F^2 + d_{ass}s_\Lambda^2 + d_{ass}s_\Lambda^2) .
$$

(3.19)

IV. EXTRAPOLATION DETAILS AND UNCERTAINTY ANALYSIS

We perform our extrapolation analysis under a Bayesian model-averaging framework as described in detail in Refs. [31, 34, 110], which is more extensively discussed for lattice QFT analysis in Ref. [56]. We consider a variety of extrapolation functions by working to different orders in the power counting, using the $l_F, s_F$ or $l_{Q1}, s_{Q1}$ small parameters, by including or excluding the chiral logarithms associated with pion loops, and by including or excluding discretization corrections scaling as $\alpha_s a^2$. The resulting Bayes factors are then used to weight the fits with respect to each other and perform a model averaging. In this section, we discuss the selection of the priors for the various LECs and then present an uncertainty analysis of the results.

A. Prior widths of LECs

In our $F_K/F_\pi$ analysis [34], we observed that using $\epsilon_a^2 = l_F^2$, $\epsilon_{\lambda}^2$ and $\epsilon_a^2$ as the small parameters in the expansion, the LECs were naturally of $O(1)$. We therefore have a prior expectation that this may hold for $w_0 m_{Q1}$ as well. The $0.12 \text{ fm}$ ensembles allow us to check this ansatz, since on this ensemble the strange quark mass was held fixed for all values of the light quark mass. We can use the a12m130 and a12m180L ensembles to estimate $c_l$ by approximating the entire shift in $w_0 m_{Q1}$ as resulting from the change in $l_F^2$ and truncating the expansion at NLO, leading to the estimate $c_l \sim 1.1$. Motivated by $SU(3)$ flavor symmetry considerations, we can roughly expect $c_s \sim c_l$. In order to be conservative, we set the prior for these LECs as

$$
\tilde{c}_l = \tilde{c}_s = N(\mu = 1, \sigma = 1) ,
$$

(4.1)

where $N(\mu, \sigma)$ denotes a normal distribution with mean $\mu$ and width $\sigma$.

Next, given these prior estimates, we can guess a prior for $c_0$ by subtracting $l_F^2$ and $s_\Lambda^2$ from $w_0 m_{Q1}$ on the a12m130 ensemble to approximate its value in the $SU(3)$ chiral limit, leading to the conservative choice

$$
\tilde{c}_0 = N(1, 1) .
$$

(4.2)

Then, we can use the difference in $w_0 m_{Q1}$ on the three ensembles with close-to-physical pion mass to estimate the leading discretization LEC in a similar manner, leading to

$$
\tilde{d}_a = N(-0.5, 1) .
$$

(4.3)

When we include the $d_a a^2 \alpha_s$ correction, since we only have four lattice spacings and we include up to $\epsilon_a^6$ corrections, we chose a value of

$$
\tilde{d}_a = N(0, 0.7) ,
$$

(4.4)

which is found to be optimal or near-optimal, as measured by the Bayes-Factor for all of the fits included in our model average. We note that the estimates we are making for the priors are significantly more conservative than the common strategy of using the effective mass to set the prior on the ground state energies.

For the higher-order priors we use

$$
\tilde{c}_l = \tilde{d}_j = N(0, 1) .
$$

(4.5)

An empirical Bayes study [55] of the prior widths leads to similar sizes for the widths. Also, as we will see, the numerical analysis does not lead to tension with the priors chosen this way.

When we use $l_{Q1}^2$ and $s_{Q1}^2$ as the small parameters instead of $l_F^2$ and $s_F^2$, we note that since $(m_{Q1}/\Lambda)^2 \sim 2$, we can use the same prescription, except to double the mean and width of all the NLO priors (which scale linearly in $l_{Q1}^2$ and $s_{Q1}^2$), set the widths to be 4 times larger for the $N^2$LO priors and 8 times larger for the $N^3$LO LECs. We do not alter the priors for the pure discretization terms, and for the mixed contributions which scale with some power of $\epsilon^2_a$ and $l_{Q1}^2$ or $s_{Q1}^2$, we increase the width of the prior based on the power of $l_{Q1}^2$ or $s_{Q1}^2$ in the term. We list the values of the priors in Table IV.

B. $w_0 m_{Q1}$ analysis and uncertainty breakdown

In order to perform the extrapolation to the continuum, infinite-volume and physical–quark-mass limits, we
consider several reasonable choices of extrapolation functions and then weight them against each other using the Bayes factor from the analysis. The various choices we consider are

- Include the ln(m_\pi) terms or counterterm only: \times 2
- Expand to N^2LO, or N^3LO: \times 2
- Include/exclude finite volume corrections: \times 2
- Include/exclude the \alpha_S a^2 term: \times 2
- Use the \Lambda = F or \Lambda = \Omega expansion: \times 2

The total choices: 32

We find that there is very little dependence upon the particular model chosen. In Fig. 6, we show the stability of the final result as various options from the above list are turned on and off. In addition, we show the impact of including or excluding the a12m220ms ensemble, whose strange quark mass is m_s \approx 0.6 \times m_{\text{phys}}^{\text{phys}}, as well as the impact of including the a06m310L ensemble. We observe a small variation of the result when either of these ensembles is dropped, but the results are still consistent with our final result (top of the figure).

The physical value of m_\Omega^{\text{phys}} is used to convert our determination of w_0m_\Omega^{\text{phys}} to a determination of w_0 at the physical point. Our final result is Eq. (1.1)

\[ w_0m_\Omega = 1.450(08)^s(05)^c(03)a(00)V(00)^{\text{phys}}(02)^M \]

\[ = 1.450(10) \]

\[ \frac{w_0}{\text{fm}} = 0.1711(09)^s(06)^c(03)a(00)V(00)^{\text{phys}}(02)^M \]

\[ = 0.1711(12) \]

with the statistical (s), chiral (\chi), continuum-limit (a), volume (V), physical-point (phys), and model selection uncertainties (M). The dominant uncertainty is statistical, suggesting a straightforward path to reducing the uncertainty to a few permil.

In Fig. 6, we also compare our result with other values of w_0 in the literature. All the results, except the most recent one from BMWc [12], have been determined in the isospin symmetric limit. Our results are in good agreement with the more recent and precise results, though one notes, there is some tension in the values of w_0 reported.

![Model breakdown](image-url)

**Fig. 6.** Model breakdown. \textbf{\chi pt-full}: \chiPT model average, including ln(m_\pi^2/\mu^2) corrections. \textbf{\chi pt-ct}: \chiPT model average with counterterms only, excluding ln(m_\pi^2/\mu^2) corrections. N^3LO/N^2LO: model average restricted to specified order. \Lambda_\chi: model average with specified chiral cutoff. incl./excl. \alpha_S: model average with/without \alpha_S corrections. excl. a06m310L: model average excluding a = 0.06 fm ensemble (a06m310L). excl. a12m220ms: model average excluding small strange quark mass ensemble (a12m220ms). Below dashed line: results from other collaborations: BMWc [2020] [12], MILC [2015] [11], HPQCD [7], QCDSF-UKQCD [2015] [8], RBC [2014] [10], HotQCD [2014] [9], BMWc [2012] [5] and ALPHA [2013] [6].

In Fig. 7, we show the resulting extrapolation of w_0m_\Omega projected into either the \ell_F^2 plane or the c_s^2 plane using the N^3LO fit including the ln(m_\pi) corrections but not including the \alpha_S a^2 corrections. The extrapolation bands are plotted in the infinite volume limit, for all other parameters held fixed except that being plotted against. For the plot versus \ell_F^2, the finite lattice spacing bands are plotted with a value of c_s^2 taken from the near-physical pion mass ensembles from Table II, a15m135XL, a12m130 and

| LEC | \Lambda = F | \Lambda = \Omega |
|-----|-------------|----------------|
| c_0 | N(1,1) | N(1,1) |
| c_{1s}, c_{s} | N(1,1) | N(2,2) |
| c_{1ls}, c_{1ls}^{in}, c_{1ls}^{in}, c_{ls}, c_{ss} | N(0,1) | N(0,4) |
| c_{1ls}, c_{1ls}^{in} | N(0,1) | N(0,8) |
| d_{ss} | N(−0.5,1) | N(−0.5,1) |
| d_{ss} | N(0.0,7) | N(0.0,7) |
| d_{ss} | N(0,1) | N(0,1) |
| d_{ss} | N(0,1) | N(0,2) |
| d_{ss} | N(0,1) | N(0,4) |

**TABLE IV.** The values of the priors used in the analysis.

![Image of Table IV](image-url)
(4.6). Such a choice leads to
\[
\frac{u_0'}{a_{15}} = 1.1432(03) \rightarrow a'_{15} = 0.1497(11) \text{ fm},
\]
\[
\frac{u_0'}{a_{12}} = 1.4155(05) \rightarrow a'_{12} = 0.12088(85) \text{ fm},
\]
\[
\frac{u_0'}{a_{09}} = 1.9450(10) \rightarrow a'_{09} = 0.08797(62) \text{ fm},
\]
\[
\frac{u_0'}{a_{06}} = 3.0119(19) \rightarrow a'_{06} = 0.05681(40) \text{ fm}. \tag{4.7}
\]

Alternatively, with our values of \( w_0/a \), we can perform a simple interpolation of these results to the physical quark mass point by utilizing the known quark mass dependence, Eq. (3.11) [81]. This interpolation can be performed for each lattice spacing separately, or in a combined analysis of all lattice spacings simultaneously. The latter is preferable in order for us to determine the lattice spacing \( a_{06} \) as we only have results at a single pion mass. To perform the global analysis, we use an N^3LO extrapolation function

\[
\frac{w_0}{a} = \frac{w_0,\text{ch}}{a} \left\{ 1 + k_l^2 + k_s + k_{a,\text{ch}} \right\} + \frac{1}{2w_0,\text{ch}/a}, \tag{4.8}
\]

This global analysis treats the value of LO parameter \( \frac{w_0,\text{ch}}{a} \) for each lattice spacing as a separate unknown parameter, and then assumes that the remaining dimensionless LECs are shared between all lattice spacings. We use this LO parameter to also construct \( \epsilon_{a,\text{ch}} \) which controls the discretization corrections rather than using \( \epsilon_a \), as \( \epsilon_{a,\text{ch}} \) is half the inverse of the left-hand-side of Eq. (4.8).

It is tempting to think of this as a combined chiral and continuum extrapolation analysis of \( w_0 \), but it is not as one normally thinks of them. Because we do not know the lattice spacings already, there remains an ambiguity in the interpretation of \( w_0,\text{ch}/a \) and the LECs \( k_a, k_{aa}, k_{la} \) and \( k_{sa} \); we are not able to interpret \( w_0,\text{ch}/a \) as the chiral limit value of \( w_0 \) divided by the lattice spacing. While the LECs accompanying the terms which are only proportional to the pure \( l_F \) and/or \( s_F \) contributions describe the quark mass dependence of \( w_0 \), here we are focussed on using this functional form to interpolate the value of \( w_0/a \) from the near-physical quark mass ensembles to the physical quark mass point.

When we perform the interpolation for each lattice spacing separately, we utilize this same expression except that we set all parameters proportional to any power of \( \epsilon_{a,\text{ch}} \) to zero. When the individual interpolations are used, the resulting values of \( a_{15}, a_{12} \) and \( a_{09} \) are compatible with those from the global analysis well within one
standard deviation

\[
\alpha = \frac{w_0/a}{a_{/\text{fm}}} \quad \text{Global} \quad \text{Individual} \quad \frac{a_{/\text{fm}}}{a_{/\text{af}}}
\]

\[
\begin{array}{llll}
\alpha_{15} & 1.1452(12) & 0.1494(11) & 1.1447(11) \\
\alpha_{12} & 1.4098(32) & 0.12134(91) & 1.4099(39) \\
\alpha_{09} & 1.9445(69) & 0.08797(70) & 1.9448(22) \\
\alpha_{06} & 2.987(15) & 0.05727(51) & 2.987(15)
\end{array}
\]

These are all in excellent agreement with Eq. (4.7) with the \( \alpha_{06} \) result being slightly more than one sigma different. Since we only have a single ensemble with \( \alpha_{06} \), this could arise from an incompletely quantified systematic uncertainty associated with determining \( \alpha_{06} \).

In Fig. 8, we show the resulting interpolation utilizing the global analysis of the values of \( w_0/a \) on all ensembles to the \( l_F^{s_{/\text{phys}}} \) and \( s_F^{s_{/\text{phys}}} \) point for each lattice spacing. The open circles show the raw values of \( w_0/a \) while the filled squares show the values shifted to \( m_0 \left( l_F^{s_{/\text{ens}}} , s_F^{s_{/\text{phys}}} , a_{/\text{ens}} \right) \) using the resultant parameters determined in the global analysis.

V. SUMMARY AND DISCUSSION

We have performed a precise scale setting with our MDWF on gradient-flowed HISQ action [13] achieving a total uncertainty of ~ 0.8% for each lattice spacing, Eq. (4.10). The scale setting was performed by extrapolating the quantity \( w_0 m_0 \left( l_F , s_F , \epsilon_a , m_\pi L \right) \) to the continuum (\( \epsilon_a \rightarrow 0 \)), infinite volume (\( m_\pi L \rightarrow \infty \)) and physical quark mass limits (\( l_F \rightarrow l_F^{s_{/\text{phys}}} \) and \( s_F \rightarrow s_F^{s_{/\text{phys}}} \)), and using the experimental determination of \( m_{11} \) to determine the scale \( w_0 \) in fm. We then interpolated our values of \( w_0/a \) to the infinite volume and physical quark mass limits for each lattice spacing, allowing for the quark-mass independent determination of \( a \) for each bare coupling \( \beta \), Eq. (4.10).

We have found that our final uncertainty is dominated by the stochastic uncertainty, Eq. (1.1), providing a clear path to reducing the uncertainty by almost a factor of 3 before needing to improve our understanding of the various systematic uncertainties. At such a level of precision, one most likely also requires a systematic study of the effect of isospin breaking on the scale setting to retain full control of the uncertainty, as has been performed by BMWc [12]. Thus, the pursuit of our physics program of determining the nucleon elastic structure functions and improving the precision of our \( g_A \) result [31, 32] will naturally lead to an improved scale setting precision. The precision we have currently is already expected to be sub-dominant for most of the results we will obtain, but a further improved precision is welcome.

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The computations were performed utilizing \textit{LALiBE} [111] which utilizes the \textit{Chroma} software suite [50] with \textit{QUDA} solvers [16, 17] and HDF5 [112] for I/O [113].
They were efficiently managed with METAQ [114, 115] and status of tasks logged with EspressoDB [116]. The HMC was performed with the MILC Code [58], and for the ensembles new in this work, running on GPUs using QUDA. The final extrapolation analysis utilized gvar v11.2 [117] and lsqfit v11.5.1 [118]. The analysis and data for this work can be found at this git repo: https://github.com/callat-qcd/project_scale_setting_mdwf_hisq.

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Appendix A: Charm quark mass reweighting

The use of reweighting [64] to estimate a correlation function with a slightly different sea-quark mass than the one simulated with is very common in LQCD, see for example Refs. [10, 119, 120]. A nice discussion of mass reweighting, including single flavor reweighting is found in Refs. [121, 122].

In our case, we are interested in reweighting the computation from the simulated charm quark mass, $m_c^{\mathrm{HMC}}$, to the physical quark mass, $m_c^{\text{phys}}$ which requires an estimate of the ratio of the fermion determinant with the physical mass to the determinant with the HMC mass. If the mass shift is a $\delta m_c = m_c^{\text{phys}} - m_c^{\mathrm{HMC}}$ then up to $O(\delta m^2)$ this ratio can be written (including the quarter-root arising from rooted-staggered fermions)

$$w_i^4 = \det [1 + \delta m (D[U_i] + m_c^{\text{phys}})^{-1}]$$  \hspace{1cm} (A1)

for each configuration $U_i$ and observables may be computed using the weight $w$,

$$\langle O \rangle_{\text{phys}} = \frac{\langle Ow \rangle_{\text{HMC}}}{(w)_{\text{HMC}}}. \hspace{1cm} (A2)$$

We can use two methods to stochastically estimate $w$ for each configuration. First, by rewriting the determinant as the exponential of a trace-log, one finds

$$w_i^4 = \exp \frac{\delta m}{4} \text{tr} [(D[U_i] + m_c^{\text{phys}})^{-1}] + O(\delta m^2)$$  \hspace{1cm} (A3)

and we can use vectors of complex Gaussian noise $\eta$ to estimate the trace,

$$\text{tr} [(D[U_i] + m_c^{\text{phys}})^{-1}] \approx \frac{1}{N_\eta} \sum_i \eta_i^\dagger \text{tr} (D[U_i] + m_c^{\text{phys}})^{-1} \eta_i,$$  \hspace{1cm} (A4)

$$\eta \sim \frac{1}{\pi} \exp -\eta^\dagger \eta. \hspace{1cm} (A5)$$

where $V$ is the size of each $\eta$ vector.

Alternatively, we may estimate the determinant in the reweighting factor (A1) using the identity

$$\det A = \pi^{-V} \int D\eta \, \eta^\dagger \, e^{-\eta^\dagger A^{-1} \eta}, \hspace{1cm} (A6)$$

which is often used to implement pseudofermions. Up to $O(\delta m^2)$, this becomes

$$w_i^4 = \pi^{-V} \int D\eta \, \eta^\dagger \, e^{-\eta^\dagger \eta} e^{\delta m \eta^\dagger \left(D[U_i] + m_c^{\text{phys}}\right)^{-1} \eta}$$  \hspace{1cm} (A7)

which tells us to draw $\eta$ according to the same gaussian (A5) and estimate

$$w_i^{\text{ps}} = \left(\frac{1}{N_\eta} \sum_j e^{\delta m \eta_j^\dagger \left(D[U_i] + m_c^{\text{phys}}\right)^{-1} \eta_j}\right)^{1/4}. \hspace{1cm} (A8)$$

Both the trace method (A3) and the pseudofermion method (A8) are only valid to $O(\delta m^2)$; when they agree we assume those corrections are under control. In order to stabilize the numerical estimate of the reweighting factors, it is also common to split the reweighting factor into a product of reweighting factors where each is computed with a fraction of the full mass shift [123–125]. For example, with a simulated mass of $m_1$ and target mass of $m_1 + \Delta m$, one could use two steps of $\Delta m/2$ and estimate the reweighting factor with the trace method,

$$w_i^{\text{tr}} = w_i^{\text{tr1}} w_i^{\text{tr2}},$$  \hspace{1cm} (A9)

$$w_i^{\text{tr1}} = \exp \frac{\Delta m/2}{4} \frac{1}{N_\eta} \sum_j \eta_j^\dagger \left(D[U_i] + m_1 + \frac{\Delta m}{2}\right)^{-1} \eta_j,$$  \hspace{1cm} (A10)

$$w_i^{\text{tr2}} = \exp \frac{\Delta m/2}{4} \frac{1}{N_\eta} \sum_j \theta_j^\dagger \left(D[U_i] + m_1 + \Delta m\right)^{-1} \theta_j,$$  \hspace{1cm} (A11)

using independently-sampled complex Gaussian noise $\eta$ and $\theta$. Of course, one may split the shift $\Delta m$ into finer steps if needed, for increased computational cost.

The reweighting factor accounts for a change in the action and is exponential in the spacetime volume. This can lead to numerical under- or overflow. As a cure, we factor out the average reweighting factor. Recognizing the trace of the inverse Dirac operator on a configuration $U_i$ as the scalar quark density times the lattice volume

$$(Vq\bar{q})_i = \text{tr} [(D[U_i] + m_q)^{-1}]$$  \hspace{1cm} (A12)
we can rescale $w$, shifting by the ensemble average $V(<cc>)$ computed via (A4). For example, rescaling the trace method (A3) gives

$$w_i^{\text{tr}} = \exp \frac{\delta m}{4} \left( \text{tr} \left[ (D[U_i] + m_c^{\text{phys}})^{-1} \right] - V(<cc>) \right); \quad (A11)$$

such a rescaling cancels exactly in the reweighting procedure (A2). A similar rescaling cures the pseudofermion method (A8). If we split the mass shift as in (A9), each factor of the weight may be independently so stabilized.

On the a06m310L ensemble the lattice volume and shift in the mass are $V = 72^3 \times 96$ and

$$\delta a_{06}m_c = a_{06}m_c^{\text{phys}} - a_{06}m_c^{\text{HMC}}$$

$$= -0.0281(4). \quad (A12)$$

While the shift in the mass is only about 10% of the physical charm quark mass, it is of the order of the physical strange quark mass. In order to stabilize the numerical estimate of the reweighting factors, we split this mass shift into 10 equal steps, and for each step, we used $N_\xi = 128$ independent Gaussian random noise vectors. For each step in the reweighting, we used the same Naik value of $\epsilon_N = -0.0533$ as was used in the original HMC. This ensures that the Dirac operator only differs from one mass to the next by the quark mass itself. As the Naik term is used to improve the approach to the continuum limit, this is a valid choice to make as it results in a slightly different approach to the continuum than if one simulated at the physical charm quark mass with the optimized Naik value for that mass.

In Fig. 9, we show the reweighting factors for each of the mass steps, with the bottom panel having a mass $a_{06}m_c = 0.28319$ closest to the HMC mass and the 2nd from top panel having $a_{06}m_c^{\text{phys}} = 0.2579$, scaled for numerical stability. The top panel is the resulting product reweighting factor normalized by the average reweighting factor. One observes that there are a few large reweighting factors of $O(100)$. We have verified that the trace estimation method (A3) and the pseudofermion method (A8) produce comparable normalized reweighting factors. The large reweighting factors are likely due to the parent HMC distribution of configurations having a suboptimal overlap with the physical, target distribution.

1. Reweighted spectrum

The next task is to understand how this reweighting impacts the extracted spectrum. To aid in this discussion, we reiterate our strategy for fitting the correlation functions. Because the noise of the omega baryon correlation function grows in Euclidean time, it is the most challenging to fit and so we focus our discussion on the omega. Our strategy is to find a good quality fit to the correlation function for which the extracted ground state energy is stable against the number of states and the time-range used in the analysis. For a given $t_{\text{min}}$, we opt to chose the simplest model which satisfies this criteria, which amounts to picking the minumum number of excited states possible.

The SS correlation functions are positive definite, therefore implying that the excited state contamination of the effective mass must come from above. When examining the SS omega-baryon effective mass on the a06m310L ensemble, one observes that around $t = 25$, the effective mass stops decreasing, and even increases a little. Because this is not allowed for a positive definite correlation function, we can conclude this must be due to a correlated stochastic fluctuation, see Fig. 10. In the reweighted effective mass, one observes more dramatic behavior of the effective mass beginning around the same time. To be conservative, we set $t_{\text{max}} = 30$ in our analysis as this allows the analysis to be sensitive to these stochastic fluctuations, which fluctuate in the opposite direction between the unweighted and reweighted configurations.

As a comparison, we also show the reweighting factors and reweighted omega baryon effective mass on the a12m130 ensemble (Fig. 11) where the charm quark was 2% different from its physical value. In this case, the reweighting factors are much easier to estimate, and we do not observe any large values.

The lower panels in Fig. 10 show the extracted ground
TABLE V. The pion, kaon and omega masses on the a06m310L ensemble with and without reweighting as well as the correlated difference.

| state  | unweighted | reweighted | difference |
|--------|------------|------------|------------|
| $m_{\pi}$ | 0.09456(06) | 0.09419(14) | -0.00037(14) |
| $m_{K}$  | 0.16204(07) | 0.16173(16) | -0.00032(15) |
| $m_{\Omega}$ | 0.5069(21) | 0.5065(29) | -0.0004(34) |

state mass as a function of $t_{\text{min}}$ and $n_{\text{state}}$. We observe that an $n_{\text{state}} = 2$ fit beginning at $t_{\text{min}} = 19$ and 15 for the unweighted and reweighted correlation functions satisfies our optimization criteria. These lead to the estimate value of $m_{\Omega}$ given in Eq. (3.7). In Table V, we also show the reweighted value of $m_{\pi}$ and $m_{K}$ on this a06m310L ensemble. While the pion and kaon have a statistically significant shift from the reweighting, when we use the reweighted values of $m_{\pi}$, $m_{K}$ and $m_{\Omega}$ from this ensemble, the final extrapolated value of $w_0 m_{\Omega}$ is within one standard deviation of the completely unweighted analysis. As the a06m310L ensemble has the largest potential change from reweighting, we conclude that at the level of precision we currently have, our results are not sensitive to the slight mistuning of the charm quark mass from its physical value on each of the configurations.

Appendix B: Models included in average

We include the results and statistics for the various models in Table VI. A few example extrapolation formula are given below to demonstrate the naming convention:

$$w_0 m_{\Omega} = c_0 + \delta_{\text{NLO}}^{\text{LO}}(l_F, s_F) + \delta_{\text{NLO}}^{\text{disc NLO}}$$

(B1a)

$$w_0 m_{\Omega} = c_0 + \delta_{\text{NLO}}^{\text{LO}}(l_F, s_F) + \delta_{\text{NLO}}^{\text{chiral NLO}} + \delta_{\text{NLO}}^{\text{disc NLO}} + \delta_{\text{NLO}}^{\text{chiral log NLO}}$$

(B1b)

$$w_0 m_{\Omega} = c_0 + \delta_{\text{NLO}}^{\text{LO}}(l_F, s_F) + \delta_{\text{NLO}}^{\text{chiral NLO}} + \delta_{\text{NLO}}^{\text{disc NLO}} + \delta_{\text{NLO}}^{\text{chiral log NLO}}$$

(B1c)

where the chiral, discretization and finite volume corrections are defined in Eqs. (3.13), (3.19) and (3.17) respectively.

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TABLE VI. Models included in final model average.

| model                                    | chi2/dof | Q    | logGBF | weight    | $w_0 m_\Omega$ | $w_0$[fm]  |
|------------------------------------------|----------|------|--------|-----------|----------------|------------|
| xpt_n3lo_alphasSF                      | 1.061    | 0.383| 65.232 | 0.080     | 1.451(11)      | 0.1712(13) |
| xpt_n3lo_F                             | 1.075    | 0.365| 65.207 | 0.078     | 1.447(09)      | 0.1708(11) |
| xpt_n3lo_FV_alphasSF                   | 1.065    | 0.378| 65.171 | 0.075     | 1.451(11)      | 0.1712(13) |
| xpt_n3lo_C                              | 1.086    | 0.353| 65.165 | 0.075     | 1.451(11)      | 0.1713(13) |
| xpt_n3lo_FV                             | 1.086    | 0.353| 65.159 | 0.075     | 1.451(11)      | 0.1713(13) |
| xpt_n3lo_FV_alphaS                      | 1.080    | 0.360| 65.144 | 0.074     | 1.447(09)      | 0.1708(11) |
| xpt_n3lo_FV_alphaS_O                    | 1.102    | 0.335| 65.130 | 0.072     | 1.448(09)      | 0.1708(10) |
| xpt_n2lo_alphaS                         | 1.101    | 0.335| 65.124 | 0.072     | 1.448(09)      | 0.1708(10) |
| xpt_n2lo_FV_alphaS                      | 1.128    | 0.306| 64.889 | 0.057     | 1.452(11)      | 0.1714(13) |
| xpt_n2lo_FV_alphaS_O                    | 1.144    | 0.289| 64.841 | 0.054     | 1.448(09)      | 0.1709(11) |
| xpt_n2lo_FV_alphaS_O_O                  | 1.132    | 0.302| 64.825 | 0.053     | 1.452(11)      | 0.1714(13) |
| xpt_n2lo_FV_alphaS_O_O_O                | 1.149    | 0.284| 64.776 | 0.051     | 1.448(09)      | 0.1709(11) |
| xpt_n2lo_FV_alphaS_O_O_O_O              | 1.165    | 0.268| 64.683 | 0.046     | 1.453(11)      | 0.1714(13) |
| xpt_n2lo_FV_alphaS_O_O_O_O_O            | 1.165    | 0.268| 64.677 | 0.046     | 1.453(11)      | 0.1714(13) |
| xpt_n2lo_FV_alphaS_O_O_O_O_O_O          | 1.183    | 0.250| 64.620 | 0.044     | 1.449(09)      | 0.1709(10) |
| xpt_n2lo_FV_alphaS_O_O_O_O_O_O_O        | 1.183    | 0.251| 64.614 | 0.043     | 1.449(09)      | 0.1709(10) |
| xpt_n3lo_FV_alphaS_O                    | 0.972    | 0.497| 59.798 | 0.000     | 1.442(12)      | 0.1701(14) |
| xpt_n3lo_FV_alphaS_O_O                  | 1.005    | 0.453| 59.767 | 0.000     | 1.442(11)      | 0.1702(13) |
| xpt_n3lo_FV_alphaS_O_O_O                | 0.970    | 0.500| 59.718 | 0.000     | 1.443(13)      | 0.1703(16) |
| xpt_n3lo_FV_alphaS_O_O_O_O              | 0.984    | 0.481| 59.704 | 0.000     | 1.442(12)      | 0.1701(14) |
| xpt_n2lo_FV_alphaS_O                    | 1.003    | 0.456| 59.686 | 0.000     | 1.444(13)      | 0.1703(16) |
| xpt_n2lo_FV_alphaS_O_O                  | 1.018    | 0.437| 59.662 | 0.000     | 1.444(11)      | 0.1702(13) |
| xpt_n3lo_FV_alphaS_O                    | 0.982    | 0.484| 59.625 | 0.000     | 1.443(13)      | 0.1703(16) |
| xpt_n2lo_FV_alphaS_O_O                  | 1.016    | 0.439| 59.582 | 0.000     | 1.444(13)      | 0.1704(16) |
| xpt_n3lo_FV_alphaS_O_O_O                | 1.130    | 0.304| 58.797 | 0.000     | 1.445(11)      | 0.1705(13) |
| xpt_n3lo_FV_alphaS_O_O_O_O              | 1.130    | 0.304| 58.796 | 0.000     | 1.445(11)      | 0.1705(13) |
| xpt_n2lo_FV_alphaS_O_O_O_O              | 1.126    | 0.308| 58.739 | 0.000     | 1.447(13)      | 0.1707(15) |
| xpt_n3lo_FV_alphaS_O_O_O_O_O            | 1.126    | 0.308| 58.738 | 0.000     | 1.447(13)      | 0.1707(15) |
| xpt_n2lo_FV_alphaS_O_O_O_O_O_O          | 1.161    | 0.272| 58.666 | 0.000     | 1.445(11)      | 0.1705(13) |
| xpt_n2lo_FV_alphaS_O_O_O_O_O_O_O        | 1.161    | 0.272| 58.655 | 0.000     | 1.445(11)      | 0.1705(13) |
| xpt_n2lo_FV_alphaS_O_O_O_O_O_O_O_O      | 1.157    | 0.276| 58.606 | 0.000     | 1.447(13)      | 0.1708(15) |
| xpt_n2lo_FV_alphaS_O_O_O_O_O_O_O_O_O    | 1.157    | 0.276| 58.605 | 0.000     | 1.447(13)      | 0.1708(15) |

Model average 1.450(10)(02) 0.1711(11)(02)
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Appendix C: Stability plots of the omega ground state mass
FIG. 12. Same as Fig. 1 for the a15m400 ensemble.

FIG. 13. Same as Fig. 1 for the a15m350 ensemble.
FIG. 14. Same as Fig. 1 for the a15m310 and a15m310L ensembles.

FIG. 15. Same as Fig. 1 for the a15m220 ensemble.
FIG. 16. Same as Fig. 1 for the a12m400 ensemble.

FIG. 17. Same as Fig. 1 for the a12m350 ensemble.
FIG. 18. Same as Fig. 1 for the a12m310 and a12m310XL ensembles.
FIG. 19. Same as Fig. 1 for the a12m220 ensembles.
FIG. 20. Same as Fig. 1 for the a12m220ms ensembles.

FIG. 21. Same as Fig. 1 for the a12m180L ensembles.

FIG. 22. Same as Fig. 1 for the a09m400 ensemble.
FIG. 23. Same as Fig. 1 for the a09m350 ensemble.

FIG. 24. Same as Fig. 1 for the a09m310 ensemble.

FIG. 25. Same as Fig. 1 for the a09m220 ensemble.