High-precision quark masses and QCD coupling
from $n_f = 4$ lattice QCD

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We present a new lattice QCD analysis of heavy-quark pseudoscalar-pseudoscalar correlators, using gluon configurations from the MILC collaboration that include vacuum polarization from $u$, $d$, $s$ and $c$ quarks ($n_f = 4$). We extract new values for the QCD coupling and for the $c$ quark’s MS mass: $\alpha_{\text{MS}}(M_Z, n_f = 5) = 0.11881(86)$ and $m_c(3 \text{ GeV}, n_f = 4) = 0.9896(69) \text{ GeV}$. These agree well with our earlier simulations using $n_f = 3$ sea quarks, vindicating the perturbative treatment of $c$ quarks in that analysis. A joint $n_f = 3$, $n_f = 4$ analysis gives improved values for the coupling and heavy-quark masses: $\alpha_{\text{MS}}(M_Z, n_f = 5) = 0.11856(53)$, $m_c(3 \text{ GeV}, n_f = 4) = 0.9864(41) \text{ GeV}$, $m_b(10 \text{ GeV}, n_f = 5) = 3.625(25) \text{ GeV}$, and $m_b/m_c = 4.54(3)$. Finally we obtain a new nonperturbative result for the ratio of $c$ and $s$ quark masses: $m_c/m_s = 11.652(65)$. This ratio implies $m_s(2 \text{ GeV}, n_f = 3) = 94.0(6) \text{ MeV}$ when it is combined with our best $c$ mass. Combining $m_c/m_s$ with our new $m_b/m_c$ gives $m_b/m_s = 52.90(44)$, which is several standard deviations away from the Georgi-Jarlskog prediction from certain GUTs.

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I. INTRODUCTION

The precision of lattice QCD simulations has increased dramatically over the past decade, with many calculations now delivering results with 1–2% errors or less. Such precision requires increasingly accurate values for the fundamental QCD parameters: the quark masses and the QCD coupling. Accurate QCD parameters are important for non-QCD phenomenology as well. For example, theoretical uncertainties in several of the most important Higgs branching fractions are currently dominated by uncertainties in the heavy-quark masses (especially $m_b$ and $m_c$) and the QCD coupling [1].

In this paper we present new lattice results for $m_c$, $m_b$, $m_c/m_s$, $m_b/m_c$, $m_b/m_s$, and $\alpha_s$. In a previous paper [2] we obtained 0.6%-accurate results for the masses and coupling by comparing continuum perturbation theory with non-perturbative lattice-QCD evaluations of current-current correlators for heavy-quark currents. Current-current correlators are particularly well suited to a perturbative analysis because non-perturbative effects are suppressed by four powers of $\Lambda_{\text{QCD}}/2m_h$ where $m_h$ is the heavy-quark mass. Our earlier simulations treated $u$, $d$ and $s$ sea quarks nonperturbatively ($n_f = 3$), while assuming that contributions from $c$ and heavier quarks can be computed using perturbation theory. Here we test the assumption that heavy-quark contributions are perturbative by repeating our analysis with lattice simulations that treat the $c$ quark nonperturbatively ($n_f = 4$ in the simulation).

In Section 2 we will present our new $n_f = 4$ lattice-QCD analysis of current-current correlators, leading to new results for the heavy-quark masses and the QCD coupling. In Section 3, we use the same simulations to calculate a new result for the ratio of the $c$ to $s$ quark masses, $m_c/m_s$. Finally, in Section 4, we summarize our conclusions, derive a new value for the $s$ mass, and present our thoughts about further work in this area. We also include, in Appendix A, a detailed discussion about how the coupling constant, quark masses, and the lattice spacing depend upon sea-quark masses in our approach. Our current analysis includes $u/d$ sea-quark masses down to physical values, so we are able to analyze this in far more detail than before.
II. LATTICE RESULTS

Our new analysis follows closely our earlier work [2]. While the lattice spacings are not as small as before, our new analysis incorporates several other improvements. The most important of these is that the new simulation treats c-quarks in the quark sea nonperturbatively. We also use the substantially more accurate HISQ discretization for the sea-quark action [3], in place of the ASQTAD discretization in our earlier analysis, and a more accurate method for setting the lattice spacing. The gluon action is also improved over our earlier analysis, as it now includes O(n_f c_s a^2) corrections [4]. Our new results also have more statistics, and include ensembles with u/d masses very close to the physical value. Finally, we use a more general parameterization (cubic splines) for the dependence of our results on the mass m_{q_h} of the pseudoscalar boson made from the heavy quark.

A. Heavy-Quark Correlator Moments

As before, we compute (temporal) moments

\[ G_n \equiv \sum_t (t/a)^n G(t) \tag{1} \]

of correlators formed from the pseudoscalar density operator of a heavy quark, j_5 \equiv i \bar{\psi}_h \gamma_5 \psi_h:

\[ G(t) = a^6 \sum_x (am_{q_h})^2 (0|j_5(x,t)j_5(0,0)|0). \tag{2} \]

Here m_{q_h} is the heavy quark’s bare mass (from the lattice QCD lagrangian), a is the lattice spacing, time t is Euclidean and periodic with period T, and the sum over spatial positions x sets the total three-momentum to zero. We again reduce finite-lattice spacing, tuning and perturbative errors by replacing the moments in our analysis with reduced moments:

\[ R_n = \begin{cases} G_4/G_4^{(0)} & \text{for } n = 4, \\ \frac{am_{q_h}}{2am_{q_h}} \left( G_n/G_n^{(0)} \right)^{1/(n-4)} & \text{for } n \geq 6, \end{cases} \tag{3} \]

where G_n^{(0)} is the moment in lowest-order weak-coupling perturbation theory using the lattice regulator, and m_{q_h} is the (nonperturbative) mass of the pseudoscalar \( h\bar{h} \) boson from the simulation.

Low-n moments are dominated by short-distance physics because the correlator is evaluated at zero total energy, which is well below the threshold for on-shell hadronic states: the threshold is at \( E_{\text{threshold}} = m_{q_h} \) where

\[ 2.9 \text{ GeV} \leq m_{q_h} < 6.6 \text{ GeV} \tag{4} \]

for our range of masses m_{q_h}. Furthermore, the moments are UV-cutoff independent when \( n \geq 4 \). Applying the Operator Product Expansion (OPE) to the product of currents in the correlator, we can therefore write our \( n = 4 \) reduced moment in terms of continuum quantities,

\[ R_4 \rightarrow r_4(\alpha_{MS}^{\text{eff}}, \mu) \left\{ 1 + \right. \]

\[ + d_4^{\text{cond}}(\alpha_{MS}^{\text{eff}}, \mu) \frac{\langle \alpha_s G^2/\pi \rangle_{\text{eff}}}{(2m_h)^4} \]

\[ + \left. d_4^{\text{cond}}(\alpha_{MS}^{\text{eff}}, \mu) \sum_{q=u,d,s} \frac{\langle m_q \bar{\psi}_q \psi_q \rangle_{\text{eff}}}{(2m_h)^4} + \cdots \right\}, \tag{5} \]

in the continuum limit (\( a \rightarrow 0 \)). Here \( \alpha_{MS}^{\text{eff}} \) and \( m_h \) are the MS coupling and h-quark mass at scale \( \mu \), respectively, and heavy-quark condensates are absorbed into the gluon condensate [5]. We will retain terms only through the gluon condensate in what follows since its contribution is already very small and contributions from other condensates will be much smaller. We discuss the precise meaning of \( \langle \alpha_s G^2/\pi \rangle_{\text{eff}} \) below. Reduced moments with \( n \geq 6 \) can be written:

\[ R_n \rightarrow z(m_{q_h}, \mu) r_n(\alpha_{MS}^{\text{eff}}, \mu) \left\{ 1 + \right. \]

\[ + d_n^{\text{cond}}(\alpha_{MS}^{\text{eff}}, \mu) \frac{\langle \alpha_s G^2/\pi \rangle_{\text{eff}}}{(2m_h)^4} + \cdots \right\} \tag{6} \]

where

\[ z(m_{q_h}, \mu) \equiv \frac{m_{q_h}}{2m_h(\mu)}. \tag{7} \]

The continuum expressions for \( R_n \) should agree with tuned lattice simulations up to finite-lattice-spacing errors of \( O((am_h)^2 \alpha_s) \). The perturbative expansions for the coefficient functions \( r_n \) are known through third order: see Table I and [6–10]. The expansions for \( d_n^{\text{cond}} \) are known through first order [11].

Parameter \( \mu \) sets the scale for \( \alpha_{MS}^{\text{eff}} \) in the perturbative expansions of the \( r_n \). As in our previous paper, we take \( \mu = 3m_h(\mu) \) in order to improve the convergence of perturbation theory. In fact, however, our method is, by design, almost completely independent of the choice of \( \mu \).

| n  | \( r_{n1} \)     | \( r_{n2} \)     | \( r_{n3} \)     |
|-----|-----------------|-----------------|-----------------|
| 4   | 0.7427          | 0.0088          | −0.0296         |
| 6   | 0.6160          | 0.4976          | −0.0929         |
| 8   | 0.3164          | 0.3485          | 0.0233          |
| 10  | 0.1861          | 0.2681          | 0.0817          |

TABLE I. Perturbation theory coefficients for \( r_n \) with \( n_f = 4 \) sea quarks, where the heaviest sea quark has the same mass \( m_{h} \) as the valence quark (that is, the quark used to make the currents in the current-current correlator). Coefficients are defined by \( r_n = 1 + \sum \mu^{1-n} \langle \alpha_s G^2/\pi \rangle_{\text{eff}}^{(\mu)} \) where \( \mu = m_h(\mu) \). These coefficients are derived in [6–10].
### B. Lattice Simulations

To extract the coupling constant and mass from simulations, we use the simulations to compute nonperturbative values for the reduced moments $R_n$ with small $n \geq 4$ and a range of heavy-quark masses $m_{Q0}$. We vary the lattice spacing, so we can extrapolate to zero lattice spacing, and the sea-quark masses, so we can tune the masses to their physical values.

The gluon-field ensembles we use come from the MILC collaboration and include $u$, $d$, $s$, and $c$ quarks in the quark sea [12, 13]. The parameters that characterize these ensembles are given in Table II. The highly accurate HISQ discretization [3] is used here for both the sea quarks and the heavy quarks in the currents used to create the correlators. This discretization was designed to minimize $(am_h)^2$ errors for large $m_h$. Our previous work used HISQ quarks in the currents, but a less accurate discretization (ASQTAD) for the sea quarks.

We also quote tuned values for the bare $s$ and $c$ quark masses in Table III. These are the quark masses that give the physical values for the $\eta_s$ and $\eta_c$ masses, as discussed in Appendix A.1.

In Table III we list our simulation results for the $\eta_s$ mass and the reduced moments for various bare quark masses $am_{Q0}$ on various ensembles. Results from different values of $am_{Q0}$ on the same ensemble are correlated; we include these correlations in our analysis. The $am_{Q0}$ values are computed from Bayesian fits of multi-state function

$$
\sum_{j=1}^{10} b_j \left( e^{-m_j t} + e^{-m_j (T-t)} \right)
$$

to the correlators $G(t)$ for $t \geq 8$, where $T$ is the temporal length of the lattice [14]. The fitting errors are small for $am_{Q0}$ and have minimal impact on our final results.

As in our previous paper, we limit the maximum size of $am_h$ (and $am_{Q0}$) in our analysis: we require $am_h \leq 0.8$. This keeps $a^2$ errors smaller than 10%.

We determine the lattice spacing by measuring the Wilson flow parameter $w_0/a$ on the lattice (Table III [15]). From previous simulations [16], we know that

$$
w_0 = 0.1715(9) \text{ fm},
$$

which we combine with our measured values of $w_0/a$ to obtain the lattice spacing for each ensemble (Appendix A). This approach is far more accurate than that used in our earlier paper, which relied upon the $r_1$ parameter from the static-quark potential.

| ensemble | $w_0/a$ | $L/a$ | $T/a$ | $N_{\text{ct}}$ | $am_{Q0}$ | $am_{Qc}$ | $am_{tuned}$ | $am_{c}$ | $\delta m_{Q0}/m_{Q0}$ | $\delta m_{Qc}/m_{Qc}$ |
|----------|---------|------|------|----------------|-----------|-----------|-------------|----------|-------------------|-------------------|
| 1        | 1.119(10) | 16   | 48   | 1020          | 0.01300   | 0.0650   | 0.383        | 0.7000(9) | 0.8897(7)        | 0.228(16)         |
| 2        | 1.127(7)  | 24   | 48   | 1000          | 0.00640   | 0.0640   | 0.828        | 0.8686(8) | 0.8717(3)        | 0.046(14)         |
| 3        | 1.136(7)  | 36   | 48   | 1000          | 0.00235   | 0.0647   | 0.831        | 0.8677(8) | 0.8607(7)        | 0.048(13)         |
| 4        | 1.382(61) | 24   | 64   | 300           | 0.01020   | 0.0509   | 0.635        | 0.5054(7) | 0.6645(3)        | 0.236(16)         |
| 5        | 1.402(9)  | 32   | 64   | 300           | 0.00507   | 0.0507   | 0.628        | 0.5033(7) | 0.6515(4)        | 0.067(14)         |
| 6        | 1.414(6)  | 48   | 64   | 200           | 0.00184   | 0.0507   | 0.628        | 0.5027(6) | 0.6435(3)        | 0.040(13)         |
| 7        | 1.933(20) | 48   | 96   | 300           | 0.00363   | 0.0363   | 0.430        | 0.0370(3) | 0.4393(4)        | 0.104(11)         |
| 8        | 1.951(7)  | 64   | 96   | 304           | 0.00120   | 0.0363   | 0.432        | 0.0364(4) | 0.4333(3)        | 0.011(13)         |
| 9        | 2.896(60) | 48   | 144  | 333           | 0.00480   | 0.0240   | 0.286        | 0.0234(3) | 0.274(2)         | 0.365(19)         |

Table III. Simulation results for $\eta_s$ masses and reduced moments with various bare heavy-quark masses $am_{Q0}$ and gluon ensembles (first column, see Table II). We do not include results from ensembles 1–3 because $am_{Q0}$ is too large for this analysis: only data for $am_{Q0} \leq 0.8$ are used here.
C. Fitting Lattice Data

Our goal is to find values for $\alpha_{\overline{\text{MS}}}^n(\mu)$ and $z(m_{\eta_b}, \mu)$ that make the theoretical results (from perturbation theory) for the reduced moments $R_n$ (Eqs. (5,6)) agree with the nonperturbative results from our simulations. We do this by simultaneously fitting results from all of our lattice spacings and quark masses for moments with $4 \leq n \leq 10$. To get good fits, we must correct the continuum formulas in Eqs. (5,6) for several systematic errors in the simulation. We fit the lattice data using the following corrected form:

\[
R_n = \begin{cases} 
1, & \text{for } n = 4 \\
m_{\eta_b}/2\xi_m m_h(\xi_m, \mu), & \text{for } n \geq 6
\end{cases}
\]

(10)

\[
x_n(\alpha_{\overline{\text{MS}}}^n(\xi_m, \mu), \mu) \times \left(1 + a_n^{\text{cond}} \left(\frac{\alpha_s G^2/\pi}{(2m_h)^4}\right)\right)
\]

(11)

\[
x_n(\alpha_{\overline{\text{MS}}}^n(\xi_m, \mu), \mu) \times \left(1 + a_n^{\text{cond}} \left(\frac{m_{\eta_b}^2 - m_{\eta_b}^2}{m_{\eta_b}^2}\right)\right)
\]

(12)

\[
\left(\frac{a_m m_{\eta_b}}{2.2}\right)^2 \sum_{i=0}^{N} c_i(m_{\eta_b}, n) \left(\frac{a_m m_{\eta_b}}{2.2}\right)^2
\]

(13)

\[
\left(\frac{a_m m_{\eta_b}}{2.2}\right)^2 \sum_{i=0}^{N} c_i(m_{\eta_b}, n) \left(\frac{a_m m_{\eta_b}}{2.2}\right)^2
\]

(14)

The values of the spline function at the knots are fit parameters, as are the derivatives at the end-points. The priors for these parameters are:

\[
\delta z(m) = 0 \pm 0.15, \quad m \in m_{\text{knots}}
\]

(15)

\[
\delta z'(m) = 0 \pm 0.30, \quad m \in \{2.9, 9.4 \text{GeV}\}
\]

(16)

\[
\text{The priors for the spline function and } z_0 \text{ are based upon results from our earlier analysis (see Fig. 6 in [2]). According to the Empirical Bayes criterion [14], the data would favor priors half as wide; so our choice is conservative. The number of knots is the smallest number that allows us to fit both our new and old data. Adding an extra knot changes our results by less than half a standard deviation and has negligible effect on the errors. The location of the knots reflects the range covered by our new data (2.9–6.6 GeV), the concentration of that data at the low-mass end of the range (hence the knot at 3.5 GeV), and our need to model behavior out to } m_{\eta_b} = 9.4 \text{GeV.}
\]

Returning to Eq. (10), it is straightforward to obtain factor $m_h(\xi_m, \mu)$ from function $z(m_{\eta_b}, \mu)$. First we calculate $m_h(\mu_0)$ at $\mu_0 = 3m_h(\mu_0)$ from

\[
m_h(\mu_0) = \frac{m_{\eta_b}}{2z(m_{\eta_b}, \mu_0)}
\]

(17)

This mass is then run perturbatively to scale $\xi_m, \mu$, where $\mu$ is calculated (iteratively) using Eq. (15). We evolve masses by integrating (numerically) the standard evolution equation:

\[
\frac{d \log m_h(\mu)}{d \log \mu} = - \gamma_0 \alpha_{\overline{\text{MS}}}^0(\mu) - \gamma_1 \alpha_{\overline{\text{MS}}}^1 - \gamma_2 \alpha_{\overline{\text{MS}}}^2
\]

\[
- \gamma_3 \alpha_{\overline{\text{MS}}}^3 - \gamma_4 \alpha_{\overline{\text{MS}}}^4
\]

(18)

Here $\gamma_0, \gamma_1, \gamma_2, \gamma_3$ are known from perturbation theory [18, 19], and $\gamma_4$ is a fit parameter with prior

\[
\gamma_4 = 0 \pm \sigma_\gamma
\]

(19)

where $\sigma_\gamma$ is the root mean square average of $\gamma_0 \cdots \gamma_3$. $\gamma_4$ has a negligible impact on our results.

2. $m_h$ Dependence

The $m_h$ mass in Eq. (10) ($n \geq 6$) comes from the simulation, while the quark mass, $m_h(\xi_m, \mu)$, is obtained from function $z(m_{\eta_b}, \mu)$ (Eq. (7)), which is one of two outputs from our fit. In our previous analysis, we parameterized $z(m_{\eta_b}, \mu)$ as a polynomial in $2\Lambda/m_{\eta_b}$. Here we use a cubic spline instead, which is more general than a polynomial: the spline assumes only that the function is smooth. Specifically we set (for $\mu = 3m_h(\mu)$)

\[
z(m, \mu) \equiv z_0 + \delta z(m)
\]

(20)

where $z_0$ is a fit parameter, with prior

\[
z_0 = 1.5 \pm 1,
\]

(21)

and $\delta z(m)$ is a cubic spline with knots at

\[
m_{\text{knots}} \equiv \{2.9, 3.5, 6.6, 9.4 \text{GeV}\}
\]

(22)

The light sea-quark masses enter linearly in $\xi_m$ and $\xi_m$, because of (nonperturbative) chiral symmetry breaking. Quark mass dependence also enters through the perturbation theory for the moments ($r_n$), but is quadratic in the mass and therefore negligible for light quarks.

3. Truncated Perturbation Theory

The Wilson coefficient function $r_n$ (Eq. (11)) has a perturbative expansion of the form

\[
r_n(\alpha_{\overline{\text{MS}}}^n, \mu) \equiv 1 + \sum_{j=1}^{N_{\mu_h}} r_{nj}(\mu) \alpha_{\overline{\text{MS}}}^j
\]

(23)
The perturbative coefficients \( r_{nj} \) are known through third order, and are given for \( \mu = m_h(\mu) \) in Table I.

The lack of perturbative coefficients beyond third order is our largest single source of systematic error. Our data are sufficiently precise that higher-order terms are relevant. Furthermore the relative importance of the higher-order terms varies with quark mass, as \( \alpha_{MS} \) varies with \( \mu = 3m_h \). Therefore we include the higher-order terms in our analysis with coefficients that we fit to account for variations with quark mass. As in our earlier analysis, we note that the known perturbative coefficients are small and relatively uncorrelated from moment to moment and order to order for \( \mu = m_h \), leading us to adopt fit priors

\[
 r_{nj}(\mu = m_h) = 0 \pm 1
\]  

(24)

for the \( n > 3 \) coefficients at \( \mu = m_h \). We double the width of these priors relative to our previous analysis because the fit suggested that some higher-order coefficients are larger here (especially for \( n = 4 \)).

We set \( N_{nth} = 15 \) terms in the expansion, although our results are essentially unchanged once 8 or more terms are included (or 5 with \( \mu = m_h \)). As before we use renormalization group equations to express the coefficients \( r_{nj}(\mu = 3m_h) \) in terms of the coefficients \( r_{nj}(\mu = m_h) \) from Table I and Eq. (24). This procedure generates (correlated) priors for the unknown coefficients at \( \mu = 3m_h \) that account for renormalization-group logarithms. The procedure makes our results largely independent of \( \mu \); our results change by less than half a standard deviation as \( \mu \) is varied over the interval \( m_h \leq \mu \leq 10m_h \).

In the fit, we parameterize \( \alpha_{MS}(\mu) \) by specifying its value at \( \mu = 5 \text{ GeV} \) with a fit parameter \( \alpha_0 \),

\[
 \alpha_{MS}(5 \text{ GeV}, n_f = 4) = \alpha_0, \tag{25}
\]

whose prior is

\[
 \alpha_0 = 0.21 \pm 0.02. \tag{26}
\]

Our previous analysis gave a result of 0.2134(24), so this is a broad prior. The coupling constant for other values of \( \mu \) is obtained by numerically integrating the evolution equation for \( \alpha_{MS}(\mu, n_f = 4) \) starting with \( \alpha_0 \) at \( \mu = 5 \text{ GeV} \):

\[
 \mu^2 \frac{d\alpha_{MS}(\mu)}{d\mu^2} = -\beta_0 \alpha_{MS}^2 - \beta_1 \alpha_{MS}^3 - \beta_2 \alpha_{MS}^4 - \beta_3 \alpha_{MS}^5 - \beta_4 \alpha_{MS}^6. \tag{27}
\]

Here \( \beta_0, \beta_1, \beta_2, \) and \( \beta_3 \) are known from perturbation theory [20, 21], and \( \beta_4 \) is a fit parameter with prior

\[
 \beta_4 = 0 \pm \sigma_\beta, \tag{28}
\]

where \( \sigma_\beta \) is the root mean square average of \( \beta_0 \ldots \beta_3 \). \( \beta_4 \) has a negligible impact on our results.

4. Nonperturbative Effects; Finite-Volume Corrections

We use the Operator Product Expansion (OPE) in Eqs. (5–6) to separate short-distance from long-distance physics. In principle, the perturbative coefficients in \( r_n(\alpha_{MS}, \mu) \) above should have subtractions coming from the higher-order terms in the OPE expansion:

\[
 r_n \rightarrow r_n \left( 1 - d_{cond}^{\text{cond}} \left( \frac{\alpha_s G^2 / \pi}{2m_h^4} \right)^n - \cdots \right) \tag{29}
\]

where \( \lambda \) is a fixed cutoff scale in the perturbative regime, say \( \lambda = 1 \text{ GeV} \), and \( \langle \alpha_s G^2 / \pi \rangle_{\text{th}}^{(n)} \) and \( d_{cond}^{\text{cond}} \) are computed in perturbation theory to the same order as \( r_n \). These subtractions come from perturbative matching, and remove contributions to \( r_n \) due to low-momentum gluons (\( \alpha \leq \lambda \)), thereby also removing infrared renormalons order-by-order in perturbation theory. The size of the subtraction depends upon the detailed definition of \( \alpha_s G^2(\lambda) \). This procedure is completely unambiguous given a specific definition for this operator, but we have not included the subtraction in \( r_n \) since it is negligible for any reasonable definition at our low orders of perturbation theory. For example, a simple momentum-space cutoff, that keeps \( q^2 < \lambda^2 \), gives \[22\]

\[
 \langle \alpha_s G^2 \rangle_{\text{th}}^{(n)} = \frac{3\alpha_s}{2\pi} \lambda^4, \tag{30}
\]

which ranges from 0.001 to 0.019 GeV\(^4\) for \( \lambda \) between 500 MeV and 1 GeV. This would change \( r_n \) by no more than 0.1–0.4% at \( m_h = m_c \) and much less at our higher \( m_h \).

Not surprisingly, perturbative estimates of the condensate value (Eq. (30)) are similar in size to nonperturbative estimates of the condensate value. So it is simpler for us to combine the subtraction in Eq. (29) with the condensate itself to form an effective condensate value [23]:

\[
 \langle \alpha_s G^2 \rangle_{\text{eff}} \equiv \langle \alpha_s G^2 \rangle_{\text{th}}^{(n)} - \langle \alpha_s G^2 \rangle_{\text{cond}}^{(n)} \tag{31}
\]

In our fits we take \( \langle \alpha_s G^2 \rangle_{\text{eff}} \) as a fit parameter with prior

\[
 \langle \alpha_s G^2 \rangle_{\text{eff}} = 0.0 \pm 0.012, \tag{32}
\]

and we approximate \( m_h \approx m_c / 2.2 \) in the condensate correction. Our results are completely unchanged if the width of this prior is ten times larger. In either case we obtain a value for the effective condensate of order 0.005 with errors of a similar size. This is completely consistent with expectations, and it reduces condensate contributions to the moments to 0.02–0.1% at \( m_h = m_c \), and much less at higher \( m_h \)—negligible at our level of precision.

This procedure is sensible at our level of precision. As precision increases, however, there is a point where it becomes important to remove renormalon corrections from the coefficients in \( r_n \). Otherwise \( j! \) factors in \( j \)th order, coming from infrared renormalons, cause perturbation theory to diverge. A simple analysis [24] indicates that perturbation theory starts to diverge at order \( j \sim 2/(\beta_0 \alpha_{MS}) \), which is around 8th order for our analysis. Consequently we expect the impact of infrared renormalons to be negligible at 3rd order.

Perturbation theory is not the whole story even if infrared renormalons are removed. The OPE separates short-distances from long-distances, but the short-distance coefficients \( r_n, d_{cond}^{\text{cond}} \ldots \) have nonperturbative contributions, for

\[
 r_n \left( 1 - d_{cond}^{\text{cond}} \left( \frac{\alpha_s G^2 / \pi}{2m_h^4} \right)^n - \cdots \right) \tag{29}
\]
example, from small instantons [22]. It is also possible that the OPE is an asymptotic expansion and does not converge ultimately, although recent results suggest it might converge [25,26]. Whatever the case, such effects are expected to appear at even higher orders than infrared renormalons, and so are completely negligible at our level of precision.

Condensates, renormalons, small instantons, etc. afflict all perturbative analyses at some level of precision. Our analysis is particularly insensitive to such effects because the leading nonperturbative contributions are suppressed by four powers of $\Lambda_{\text{QCD}}/(2m_b)$.

Note finally that the coefficient functions, being short-distance, are insensitive to errors caused by the finite volume of the lattice. While the finite volume can affect the value of $\langle\alpha_s G^2\rangle_{\text{eff}}$, the impact on our results is negligible since the condensate itself is negligible. Finite-volume corrections are also negligible in our determinations of $m_{\eta_c}$. Simulation data in [27] shows finite-volume effects in $m_{\eta_c}$ of order 0.05%; they will be much smaller for $m_{\eta_b}$. Additional evidence comes from [28] which shows that finite-volume effects are less than 0.02% for the $D_s$ mass.

5. $m_{\eta_b} - m_{\eta_c}$ Correction

Our results are also affected by the difference between the $c$ mass $m_{\eta_c}$ used in the sea, and the mass of the heavy quark $m_{\eta_b}$ used to make the currents in the current-current correlator. The perturbative calculations we use assume $m_{\eta_c} = m_{\eta_b}$, but we want to study a range of $m_{\eta_b}$ values with fixed $m_{\eta_c}$. The correction enters in $O(\alpha_s^2)$, is quadratic in the mass difference for small differences, and goes to a (small) constant as $m_{\eta_b} \to \infty$. Therefore we correct for it using (Eq. 13)

$$R_n \to R_n \left(1 + \delta R_n \right)$$  (33)

where $h_n$ is a fit parameter with a prior of $0 \pm 0.03$. The width 0.03 is ten times larger than the correct value from perturbation theory in the $m_{\eta_b} \to \infty$ limit. It is twice as wide as the width indicated by the Empirical Bayes criterion [14]. We also tried fits where $d_\alpha^{n,c}$ was replaced by a spline function of $m_{\eta_b}$. These give similar results but with larger errors (especially for $\alpha_{\text{MS}}$).

6. Finite Lattice Spacing Errors

The final modification in our formula for $R_n$ corrects for errors caused by the finite lattice spacings used in the simulations. We write

$$R_n \to R_n + \delta R_n$$  (34)

where

$$\delta R_n = \left(\frac{a m_{\eta_b}}{2.2}\right)^2 \sum_{i=0}^{N} c_i^{(n)}(m_{\eta_b}) \left(\frac{a m_{\eta_b}}{2.2}\right)^{2i}$$  (35)

and $m_{\eta_b}/2.2$ is a proxy for the quark mass. The $c_i^{(n)}(m_{\eta_b})$ are again cubic splines, using the same knots as used for $z(m_{\eta_b}, \mu)$ (Eq. 18). As before, we set

$$c_i^{(n)}(m) = c_i^{(n)}(m) + \delta c_i^{(n)}(m)$$  (36)

with the following fit parameters and priors:

$$c_i^{(n)}(m) = 0 \pm 1/n$$

$$\delta c_i^{(n)}(m) = 0 \pm 0.15/n \quad m \in m_{\text{knots}}$$

$$\delta c_i^{(n)}(m) = 0 \pm 0.30/n \quad m \in \{2.9, 9.4 \text{GeV}\}.$$  (37)

These priors are again conservative since the Empirical Bayes criterion [14] suggests priors that are half as wide. We take $N = 20$ but our results are insensitive to any $N \geq 8$.

7. Physics

We calculate results on ensembles with different lattice spacings, ranging between 0.12 fm and 0.06 fm, and various sea-quark masses, with $u$, $d$, $s$ and $c$ quarks in the sea. The extrapolated results are then compared with the perturbative predictions (Eqs. 5–6) with $\mu = 3m_{\eta_c}$ as in our previous work. The coupling $\alpha_{\text{MS}}$ and function $z$ are adjusted by the fit so that the perturbative expressions agree with the (nonperturbative) results from the simulations. Finally the $c$-quark mass is obtained from $z$ and the physical value for the $\eta_c$ mass:

$$m_c(3m_c) = \frac{m_{\eta_c}^{\text{phys}}}{2z(m_{\eta_c}^{\text{phys}}, 3m_c)}.$$  (38)

As discussed in Appendix A.1 we adjust the physical $\eta_c$ mass (and its error) in this equation to account for electromagnetic effects and $c\bar{c}$ annihilation, neither of which is included in our simulation. This is the most important correction for electromagnetism in our analysis; other electromagnetic effects are negligible at our level of precision.

D. $n_f = 4$ Lattice Results

We fit all of the reduced moments from our simulation data—with lattice spacings from 0.12 fm to 0.06 fm, and $n = 4, 6, 8$ and 10 in Table III—simultaneously to formula (10–14) by adjusting fit parameters described in the previous sections. The fit is excellent with a $\chi^2$ per degree of freedom of 0.39 for 92 pieces of data ($p$-value is 1.0).

The fit has two key physics outputs. One is a new result for the running coupling constant:

$$\alpha_{\text{MS}}(5\text{GeV}, n_f = 4) = 0.2148(29).$$  (39)

To compare with our old determination and other determinations, we use perturbation theory to add $b$ quarks to the sea [29], with $m_b(m_t) = 4.164(23)\text{GeV}$ [2], and evolve to the $Z$ mass (91.19 GeV) to get

$$\alpha_{\text{MS}}(M_Z, n_f = 5) = 0.11881(86).$$  (40)
This agrees well with 0.1183(7) from our $n_f = 3$ analysis [2]. It also agrees well with the current world average 0.1185(6) from the Particle Data Group [30].

The second important physics output is the mass-ratio function $z(m_{Qb}, \mu)$. This function equals 1.506(6) when evaluated at $m_{Qb}^{hys}$ with $\mu = 3m_c$. We obtain results for the $c$ mass by substituting this value into Eq. (38) and using perturbation theory (Eq. (41)) to evolve to various scales:

$$m_c(\mu, n_f = 4) = \begin{cases} 0.9915(57) \text{ GeV} & \mu = 3m_c \\ 0.9886(69) \text{ GeV} & \mu = 3 \text{ GeV} \\ 1.281(11) \text{ GeV} & \mu = m_c. \end{cases}$$

(41)

These agree to within a standard deviation with our previous $n_f = 3$ analysis [2], which gave 0.986(6) GeV for the mass at 3 GeV. There is relatively little correlation between our estimates for $m_c(3 \text{ GeV})$ and $\alpha_{MS}(M_Z)$: the correlation coefficient is 0.13.

Our result at $\mu = m_c$ has a larger error because $\alpha_{MS}$ in the mass evolution equation (Eq. (21)) becomes fairly large at that scale ($\alpha_{MS} \approx 0.4$) and quite sensitive to uncertainties in its value. We use the coupling from our fit for this evolution. Were we instead to use the Particle Data Group’s (more accurate) $\alpha_{MS}$, our value for $m_c(m_c)$ would be 1.278(8) GeV. In any case, it is probably better to avoid such low scales, if possible.

We can also compare our new results with our previous work for quark masses larger than $m_c$. This is done in Fig. 1. Again agreement is good at the 1σ level. Our new fit has little predictive value above $m_{Qb} \approx 6.6 \text{ GeV}$ because we have no data beyond that point.

Our results confirm that a perturbative treatment of $c$ quarks in the sea, as in our previous paper, is correct, at least to our current level of precision.

| $m_c(3)$ | $\alpha_{MS}(M_Z)$ | $m_c/m_s$ |
|----------|-------------------|-----------|
| Perturbation theory | 0.3 | 0.6 | 0.0 |
| Statistical errors | 0.3 | 0.2 | 0.3 |
| $a^2 \to 0$ extrapolation | 0.3 | 0.4 | 0.0 |
| $\delta m_{uds}$ | 0.2 | 0.0 | 0.0 |
| $\delta m_{c}$ | 0.3 | 0.1 | 0.0 |
| $m_h \neq m_c$ correction (Eq. (13)) | 0.1 | 0.0 | 0.0 |
| Uncertainty in $w_0, w_0/a$ | 0.2 | 0.1 | 0.1 |
| $\alpha_0$ prior | 0.0 | 0.1 | 0.0 |
| Uncertainty in $m_{Qb}$ | 0.0 | 0.0 | 0.4 |
| $\delta m_{Qb}$: electromag., annih. | 0.1 | 0.0 | 0.1 |
| Total: | 0.70% | 0.72% | 0.55% |

(41)

TABLE IV. Error budget [31] for the $c$ mass, QCD coupling, and the ratio of quark masses $m_c/m_s$ from the $n_f = 4$ simulations described in this paper. Each uncertainty is given as a percentage of the final value. The different uncertainties are added in quadrature to give the total uncertainty. Only sources of uncertainty larger than 0.05% have been listed.

The dominant sources of error for our results are listed in Table IV. The most important systematics are due to the truncation of perturbation theory and to our extrapolation to $a^2 = 0$. Statistical errors are also important. As in our previous analysis, the $a^2$ extrapolations are not large, as is clear from Figure 2. Also the dependence of our results on the light sea-quark masses is quite small and independent of the lattice spacing, as illustrated by Figure 3.

Our results change by less than $\sigma/2$ if we fit only the $n = 4$ and 6 moments, but the errors are 10–40% larger (especially for the $c$ mass). Leaving out $n = 4$, instead, more than doubles the error on $\alpha_{MS}(M_Z)$. We limit our analysis to heavy quark masses with $am_{Qb} \leq 0.8$, as in our previous analysis. Reducing that limit to 0.7, for example, has no impact on the central values of results and increases our errors only slightly (less than 10%).

We tested the reliability of our error estimates for the perturbation theory by refitting our data using only a subset of...
FIG. 3. Light sea-quark mass dependence of reduced moments $R_n$ for $m_h = m_c$, and $n = 4, 6, 8, 10$. Results are shown for our two coarsest lattices: $a = 0.12$ fm (three points in blue) and $a = 0.09$ fm (two points in red). The dashed lines show the corresponding results from our fit. Note that the slopes of the lines are independent of the lattice spacing, as expected.

the known perturbative coefficients. The results are presented in Fig. 4 which shows values for $m_c(3 \text{ GeV})$ and $\alpha_{\text{MS}}(M_Z)$ from fits that treat perturbative coefficients beyond order $N$ as fit parameters, with priors specified by Eq. (24). The gray bands and dashed lines indicate the means and standard deviations of our final results, which correspond to $N = 3$.

higher-order coefficients.

E. Joint $n_f = 3$, $n_f = 4$ Results

Our earlier $n_f = 3$ analysis [2] is more accurate than our new analysis because it includes results from a smaller lattice spacing (0.045 fm). The smaller lattice spacing also allowed us to include the $b$ mass in that analysis. These earlier results can be further improved by combining them with the new $n_f = 4$ data described in this paper. Our ability to successfully fit both sets of data simultaneously provides an additional test of the validity of each data set, and the reliability of the perturbative treatment of $c$ sea quarks used in the earlier analysis.

To merge our $n_f = 3$ and $n_f = 4$ results, we use the old code to generate predictions for $m_h(\mu = 3m_h,n_f = 4)$ at several values of $m_{\eta_h}$: 2.98, 4.6, 6.2, 7.8 and 9.4 GeV. We then include these results in our new analysis as additional data, to be fit by our formalism. In addition we use the old code to generate a prediction for $\alpha_{\text{MS}}(5 \text{ GeV}, n_f = 4)$ and use that value for the $\alpha_0$ prior, instead of Eq. (26). In a Bayesian framework, this composite fit is approximately equivalent to a joint fit of the $n_f = 3$ and $n_f = 4$ data sets.

The joint fit is excellent, with a $\chi^2$ per degree of freedom of 0.49 for 97 degrees of freedom ($p$-value of 1.0). The $c$-quark mass from the joint fit is

$$m_c(\mu, n_f = 4) = \begin{cases} 0.9864(41) \text{ GeV} & \mu = 3 \text{GeV} \\ 1.2758(58) \text{ GeV} & \mu = m_c, \end{cases}$$

which agrees with the separate analyses to better than a standard deviation. The joint fit also gives new results for the

These are somewhat lower than our previous $n_f = 3$ values. The differences are consistent with perturbation theory, though a definitive comparison would require fourth and
and masses of our entire analysis. Agreement provides a highly non-trivial check on the validity of the completely nonperturbative result, 4.49(4), from \[2\]. The perturbative result agrees well with the independent, correlated than in the joint fit results from our previous \((n_f = 3)\) analysis, corrected to \(n_f = 4\) using perturbation theory.

This perturbative result agrees well with the independent, completely nonperturbative result, 4.49(4), from \[2\]. The agreement provides a highly non-trivial check on the validity of our entire analysis.

III. \(m_c/m_s\) FROM \(n_f = 4\)

We can use lattice QCD to extract ratios of \(\overline{\text{MS}}\) quark masses completely nonperturbatively \[32\], since ratios of quark masses are scheme and scale independent: for example,

\[
\frac{m_{QC}/m_{0s}}{m_{0s}/\text{lat}} = \frac{m_c(\mu, n_f)}{m_s(\mu, n_f)}_{\overline{\text{MS}}} + \mathcal{O}((am_c)^2 \alpha_s).
\]

While ratios of light-quark masses can be obtained from chiral perturbation theory, only lattice QCD can produce nonperturbative ratios involving heavy quarks. These ratios are very useful for checking mass determinations that rely upon perturbation theory, as discussed in Section [11]. They also allow us to leverage precise values of light-quark masses from very accurately determined heavy-quark masses.

In \[32\] we used nonperturbative simulations, with \(n_f = 3\) sea quarks, to determine the \(s\) quark’s mass from the \(c\) quark’s
mass and the ratio $m_c/m_s$. We repeat that analysis here, but now for $n_f = 4$ sea quarks, using the tuned values of the bare $s$ and $c$ masses for each of our lattice ensembles: $am_{0,\text{tuned}}$ and $am_{0,\text{tuned}}$ in Table 11 respectively. We expect

\[
\frac{am_{0,\text{tuned}}}{am_{0,\text{tuned}}} = \frac{m_c}{m_s} \left( 1 + h_m \frac{\delta m^\text{sea}}{m_s} + h_{a^2,m} \frac{\delta m^\text{sea}}{m_s} \left( \frac{m_c}{\pi/a} \right)^2 \right. \\
+ \left. h_1 \alpha_s(\pi/a) \left( \frac{m_c}{\pi/a} \right)^2 + \sum_{j=2}^{N_f^2} h_j \left( \frac{m_c}{\pi/a} \right)^{2j} \right),
\]

(48)

where again we ignore $\delta m^\text{sea}$ and $\delta m^2$ dependence since they are negligible. We fit the data from Table 11 using this formula with the following fit parameters and priors:

\[
h_m = 0 \pm 0.1, \quad h_{a^2,m} = 0 \pm 0.1, \quad h_1 = 0 \pm 6, \quad h_j = 0 \pm 2 \quad (j > 1).
\]

(49, 50)

The extrapolated value $m_c/m_s$ is also a fit parameter. We set $N_f = 5$, but get identical results for any $N_f^2 \geq 2$.

The result of this fit is presented in Fig. 6 which shows the $a^2$ dependence of the lattice results. The sensitivity of our new results to $a^2$ is about half what we saw in our previous analysis. Our new fit is excellent and gives a final result for the mass ratio of:

\[
\frac{m_c(\mu, n_f)}{m_s(\mu, n_f)} = 11.652(65).
\]

(51)

The leading sources of error in this result are listed in Table IV. These are dominated by statistical errors and uncertainty in the $\eta_b$ mass. Many other potential sources of error, such as uncertainties in the lattice spacing, cancel in the ratio.

Our result is about two standard deviations lower than the recent result, 11.747(19) ($+^{59}_{-41}$), computed by the Fermilab/MILC collaboration (using many of the same configurations we use) 28]. Our analysis uses a different scheme for tuning the lattice spacing and quark masses, which results in essentially no dependence on the sea-quark masses for $m_c/m_s$. The absence of sea-mass dependence is apparent from Fig. 3 where the clusters of data points correspond to ensembles with the same bare lattice coupling but different sea-quark masses. This figure can be compared with Fig. 6 in 28], which shows much larger sea-mass dependence. Both approaches should agree if extrapolated to zero lattice spacing and the physical sea-quark masses.

IV. CONCLUSIONS AND OUTLOOK

The initial extractions of quark masses from heavy-quark current-current correlators relied upon experimental data from $e\pi$ annihilation 33, 34]. Our analysis here, like the two that preceded it 2, 35], replaces experimental data with nonperturbative results from tuned lattice simulations.

Lattice simulations offer several advantages over experiment for this kind of calculation 11]. For one thing, simulations are easier to instrument than experiments and much more flexible. Thus we can generate lattice “data” not just for vector-current correlators, but for any heavy-quark current or density; we optimize our simulations by using the pseudoscalar density instead of the vector current. Experiment provides results for only two heavy-quark masses — $m_c$ and $m_b$ — but we can produce lattice data for a whole range of masses between $m_c$ and $m_b$. This means that $\alpha_{\text{MS}}(\mu)$ varies continuously, by almost a factor of two, in our analysis since $\mu \propto m_h$. Here we use this variation to estimate and bound uncalculated terms in perturbation theory, providing much more reliable estimates of perturbative errors than the standard procedure of replacing $\mu$ by $\mu/2$ and $2\mu$. (Our analysis is essentially independent of $\mu$.) Nonperturbative contributions are also strongly dependent upon $m_h$, and therefore more readily bound if a range of masses is available; they are negligible in our analysis.

In this paper, we have redone our earlier $n_f = 3$ analysis 2 using simulations with $n_f = 4$ sea quarks: $u, d, s$ and $c$. Our new results,

\[
m_c(3 \text{ GeV}, n_f = 4) = 0.9896(69) \text{ GeV},
\]

(52)

\[\alpha_{\text{MS}}(M_Z, n_f = 5) = 0.11881(86),\]

(53)

agree well with our earlier results of 0.986(6) GeV and 0.1183(7), suggesting that contributions from $c$ quarks in the sea are reliably estimated using perturbation theory (as expected). Our $c$ mass is about 1.4$\sigma$ lower than the recent result from the ETMC collaboration, also using $n_f = 4$ simulations but with a different method 36]: they get $m_c(\mu_c) = 1.348(42)$ GeV, compared with our $n_f = 4$ result of 1.281(11) GeV.

We have also done a joint analysis, combining our new $n_f = 4$ data with our earlier $n_f = 3$ data, to obtain results that are more accurate than our earlier results:

\[
m_c(3 \text{ GeV}, n_f = 4) = 0.9864(41) \text{ GeV},
\]

(54)

\[
m_b(10 \text{ GeV}, n_f = 5) = 3.625(25) \text{ GeV},
\]

(55)

\[
m_b/m_c = 4.54(3),
\]

(56)

\[
\alpha_{\text{MS}}(M_Z, n_f = 5) = 0.11856(53).
\]

(57)

The excellent fit is further evidence that the two sets of data are consistent with each other when $c$ quarks in the sea are treated perturbatively.

Finally, we updated our earlier $n_f = 3$ analysis 32 of the ratio $m_c/m_s$ of quark masses using our $n_f = 4$ data. This is a relatively simple analysis of data from Table 11. Our new value is:

\[
\frac{m_c(\mu, n_f)}{m_s(\mu, n_f)} = 11.652(65).
\]

(58)

It agrees well with our previous result 11.85(16), but is much more accurate. We compare our results with others in Fig. 7.

We obtain a new estimate for the $s$ mass by combining our new result for $m_c/m_s$ with our best estimate of the $c$ mass (Eq. 54):

\[
m_s(\mu, n_f = 3) = \begin{cases} 94.0(6) \text{ MeV} & \mu = 2 \text{ GeV} \\ 84.9(6) \text{ MeV} & \mu = 3 \text{ GeV}. \end{cases}
\]

(59)
Values for $m_s(\mu, n_f = 4)$ are smaller by about 0.2 MeV. Our new result agrees with our previous analysis and also with other recent $n_f = 3$ or 4 analyses:

\[
m_s(2\text{GeV}) = \begin{cases} 
92.4(1.5)\text{MeV} & \text{HPQCD [32]}, \\
99.6(4.1)\text{MeV} & \text{ETMC [36]}, \\
95.5(1.9)\text{MeV} & \text{Durr et al. [39]}, 
\end{cases}
\]

\[
m_s(3\text{GeV}) = 83.5(2.0)\text{MeV} \quad \text{RBC/UKQCD [40]}. \quad (60)
\]

We can also use this ratio with our new value for $m_b/m_c$ to obtain the ratio of the $b$ to $s$ masses,

\[
\frac{m_b(\mu, n_f)}{m_s(\mu, n_f)} = 52.90(44). \quad (61)
\]

This is several standard deviations away from the result predicted by the Georgi-Jarlskog relationship [41] for certain classes of grand unified theory: the Georgi-Jarlskog relationship says that $m_b/m_s$ should equal $3m_s/m_u = 50.45$.

The prospects for improving our results over the next decade are good. Detailed simulations, described in [1], indicate that errors from our analysis can be pushed below 0.25% by a combination of higher-order perturbation theory, and, especially, smaller lattice spacings (0.045, 0.03 and 0.023 fm) — both improvements that are quite feasible over a decade [1]. There are also many other promising approaches within lattice QCD. Several exist already for extracting the QCD coupling: see, for example, [42, 47].

In this appendix we discuss the dependence of the $\overline{\text{MS}}$ coupling and heavy-quark masses on the sea-quark masses. We vary the $u/d$ sea-quark mass in our simulations to help us assess systematic errors associated with tuning that mass. In addition, the precision with which the $s$ and $c$ sea-quark masses have been tuned varies by several percent over the various ensembles we use. These detunings shift the $\overline{\text{MS}}$ coupling and masses. We need to understand how they are shifted in order to extract results for $\alpha_{\overline{\text{MS}}}$ and $m_b$ with physical sea-quark masses.

Lattice simulations are done for particular values of the bare coupling constant (and bare quark masses), but with all dimensional quantities expressed in units of the lattice spacing (lattice units). This removes explicit dependence on the lattice spacing from the simulation, so we can run the simulation without knowing the lattice spacing. To extract physics, however, we must determine the lattice spacing (from the simulation) and convert all simulation results from lattice units to physical units. In our simulations, we calculate the lattice spacing by measuring the value of $a/w_0$ in the simulation, and multiplying it by the known value of $w_0$ for physical sea-quark masses (that is, 0.1715(9) fm). As a result the lattice spacing becomes (weakly) dependent upon the sea-quark masses since $w_0$ is affected by sea quarks.

This procedure is convenient because the lattice spacing for a given ensemble is determined using information from only that ensemble, thereby decoupling the analyses of different ensembles to a considerable extent. As we discuss below there is an added benefit when vacuum polarization from $c$ (or heavier) quarks is included in the simulation, as we do here: heavy quarks automatically decouple from low-energy physics (like $w_0$ [51]). With our procedure, physical quantities that probe energy scales smaller than $2m_c$ — that is, almost everything studied with lattice QCD today — are essentially independent of $m_c$, which means that they are completely unaffected by tuning errors in $m_c$. This would not be the case if we fixed the

\[
\text{ACKNOWLEDGMENTS}
\]

We are grateful to the MILC collaboration for the use of their gauge configurations and code. We thank S. King and D. Toussaint for useful conversations. Our calculations were done on the Darwin Supercomputer as part of STFC’s DiRAC facility jointly funded by STFC, BIS and the Universities of Cambridge and Glasgow. This work was funded by STFC, the Royal Society, the Wolfson Foundation and the National Science Foundation.

Appendix A: Sea-Quark Mass Dependence

FIG. 7. Lattice QCD determinations of the ratio of the $c$ and $s$ quarks’ masses. The ratios come from this paper and references [28, 32, 36-38]. The gray band is the weighted average of the three $n_f = 4$ results: 11.700(46).

There are also many other promising approaches within lattice QCD. Several exist already for extracting the QCD coupling and heavy-quark masses on the sea-quark masses. We find it more convenient, however, to explore a slightly different manifold in theory space by fixing $\alpha_{\text{lat}}$ and the value of the Wilson-flow parameter $w_0$. Lattice simulations are done for particular values of the bare coupling constant (and bare quark masses), but with all dimensional quantities expressed in units of the lattice spacing (lattice units). This removes explicit dependence on the lattice spacing from the simulation, so we can run the simulation without knowing the lattice spacing. To extract physics, however, we must determine the lattice spacing (from the simulation) and convert all simulation results from lattice units to physical units. In our simulations, we calculate the lattice spacing by measuring the value of $a/w_0$ in the simulation, and multiplying it by the known value of $w_0$ for physical sea-quark masses (that is, 0.1715(9) fm). As a result the lattice spacing becomes (weakly) dependent upon the sea-quark masses since $w_0$ is affected by sea quarks.

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lattice spacing instead of \( w_0 \), since it is small variations in the lattice spacing that correct for mistuning in \( m_c \).

It is also very convenient that we set the lattice spacing using a flavor singlet quantity. Because \( w_0 \) is a flavor singlet, the leading sea-mass dependence induced in the lattice spacing is analytic (linear) in the quark mass and small; in particular, there are no chiral logarithms \([52]\). One consequence is that leading-order chiral perturbation theory for physical quantities (\( f_\pi, f_D, \ldots \)) is unchanged from standard treatments except for shifts (that are easily accommodated) in the coefficients of certain analytic terms.

In this appendix we show how the \( \overline{\text{MS}} \) coupling and heavy-quark mass depend upon the sea-quark masses in our simulations. This dependence implies sea-quark mass dependence in the lattice spacing and the heavy quark’s bare mass, which we then use to determine some of the parameters involved. Finally we review heavy-quark decoupling, and estimate the parameters for \( c \)-mass dependence using first-order perturbation theory.

### 1. Tuning Bare Quark Masses

We define tuned values for the bare \( c \) and \( s \) masses on each ensemble by adjusting those masses to give physical values in simulations for the \( \eta_c \) and \( \eta_s \) masses. The tuned values are listed in Table II.

The current experimental value for the \( \eta_c \) mass is 2.9837(7) GeV \([30]\). In our analysis, we remove electromagnetic corrections from this value, and adjust its error to account for \( \pi \pi \) annihilation, since neither effect is in our simulations \([53, 54]\). We use:

\[
m_{\eta_c}^{\text{phys}} = 2.9863(27) \text{ GeV}.
\]

We compute the tuned \( c \) mass \( a m_{\eta_c}^{\text{tuned}} \) by linear interpolation using \( \eta_c \) masses from the simulation (Table III) for heavy-quark masses \( m_{\eta_c} \) in the vicinity of \( m_{\eta_c} \). In a few cases we have results for only a single value of \( m_{\eta_c} \); then we compute the tuned \( c \) mass using estimates of \( dm_{\eta_c}/dm_{\eta_c} \) from other ensembles with (almost) the same lattice spacing.

The \( \eta_s \) is an \( s\bar{s} \) pseudoscalar particle where the valence quarks are (artificially) not allowed to annihilate; its physical mass is determined in lattice simulations from the masses of the pion and kaon \([16]\):

\[
m_{\eta_s}^{\text{phys}} = 0.6885(22) \text{ GeV}
\]

This mass is defined for use in lattice simulations and needs no further corrections for electromagnetism. We tune the \( s \) mass by simulating with a nearby bare mass \( a m_s \) to obtain the corresponding \( \eta_s \) mass, and then extracting the tuned mass using:

\[
am_{\eta_s}^{\text{tuned}} = a m_s \left( \frac{m_{\eta_s}^{\text{phys}}}{m_{\eta_s}} \right)^2.
\]

Our \( \eta_s \) data are presented in Table IV, which shows that the tuned mass is quite insensitive to small variations in \( a m_{\eta_s} \).

| ensemble | \( a m_{\eta_s} \) | \( a m_{\eta_s} \) | \( a m_{\eta_s}^{\text{tuned}} \) |
|----------|----------------|----------------|-----------------|
| 1        | 0.0705         | 0.54024(15)   | 0.0700(9)       |
| 2        | 0.0688         | 0.53350(17)   | 0.0700(9)       |
| 3        | 0.0641         | 0.51511(16)   | 0.0700(9)       |
| 4        | 0.0679         | 0.52798(9)    | 0.0686(8)       |
| 5        | 0.0636         | 0.51080(9)    | 0.0687(8)       |
| 6        | 0.0678         | 0.52680(8)    | 0.0677(8)       |
| 7        | 0.0541         | 0.43138(12)   | 0.0543(7)       |
| 8        | 0.0522         | 0.42358(11)   | 0.0545(7)       |
| 9        | 0.0533         | 0.42637(6)    | 0.0533(7)       |
| 10       | 0.0507         | 0.41572(14)   | 0.0534(7)       |
| 11       | 0.0505         | 0.41474(8)    | 0.0534(7)       |
| 12       | 0.0527         | 0.42310(3)    | 0.0527(6)       |
| 13       | 0.0507         | 0.41478(4)    | 0.0527(6)       |
| 14       | 0.0536         | 0.30480(4)    | 0.0364(4)       |
| 15       | 0.0231         | 0.20549(8)    | 0.0234(3)       |

We do not have \( \eta_s \) results for ensemble 7; there the tuned \( s \) mass is based on an interpolation between results from ensemble 8 and another ensemble that has similar parameters but with \( a m_{\eta_s} = 0.0074 \).

We set the \( u \) and \( d \) masses equal to their average,

\[
m_\ell \equiv \frac{m_u + m_d}{2},
\]

and set \( m_\ell \) equal to the tuned \( s \) mass (above) times the physical value of the quark mass ratio \([28]\)

\[
m_s/m_\ell = 27.35(11).
\]

### 2. \( \alpha_{\overline{\text{MS}}}(\mu, \delta m^{\text{sea}}) \) and \( a(\delta m^{\text{sea}}) \)

The beta function in the \( \overline{\text{MS}} \) scheme is, by definition, independent of sea-quark masses. Thus the coupling’s evolution is unchanged by detuned sea-quark masses —

\[
\frac{d \alpha_{\overline{\text{MS}}} (\mu, \delta m^{\text{sea}})}{d \log \mu^2} = \beta (\alpha_{\overline{\text{MS}}} (\mu, \delta m^{\text{sea}}))
\]

— but mass dependence enters through the low-energy starting point for that evolution implied by the scale-setting procedure used in the lattice simulation. Such mass dependence can enter only through an overall renormalization of the scale parameter \( \mu \):

\[
\alpha_{\overline{\text{MS}}} (\mu, \delta m^{\text{sea}}) = \alpha_{\overline{\text{MS}}} (\xi_0 \mu)
\]

where

\[
\alpha_{\overline{\text{MS}}} (\mu) = \alpha_{\overline{\text{MS}}} (\mu, \delta m^{\text{sea}} = 0)
\]
is the \( \overline{\text{MS}} \) coupling for physical sea-quark masses. The scale factor,

\[
\xi_\alpha \equiv 1 + g_\alpha \frac{\delta m_{\text{uds}}^{\text{sea}}}{m_s} + g_{a^2,\alpha} \frac{\delta m_{\text{uds}}^{\text{sea}}}{m_s} \left( \frac{m_c}{\pi/a} \right)^2 \\
+ g_{c,\alpha} \frac{\delta m_{\text{sea}}^{\text{sea}}}{m_c} + O(\delta m^2),
\]

(A9)

depends upon the differences between the masses \( m_q \) used in the simulation and the tuned values of those masses \( m_q^{\text{tuned}} \) (Table II and Sec. A1):

\[
\delta m_{\text{uds}}^{\text{sea}} \equiv \sum_{q=u,d,s} (m_q - m_q^{\text{tuned}})
\]

(A10)

\[
\delta m_{c}^{\text{sea}} \equiv m_c - m_c^{\text{tuned}}.
\]

(A11)

Function \( \alpha_{\overline{\text{MS}}}^{\text{sea}}(\xi_\alpha, \mu) \) satisfies the standard evolution equation (Eq. (A6)) because \( \xi_\alpha \) is independent of \( \mu \).

We work to first order in \( \delta m^{\text{sea}} \) because higher-order terms are negligible in our simulations. As suggested above, the leading-order dependence is particularly simple because we use iso-singlet mesons (\( \eta_c \) and \( \eta_s \)) to set the \( c \) and \( s \) masses; in particular, there are no chiral logarithms of the \( u/d \) mass in leading order.

We expect coefficients \( g_\alpha \) and \( g_{a^2,\alpha} \) in \( \xi_\alpha \) to be of order 1/10 since corrections linear in light-quark masses must be due to chiral symmetry breaking and so should be of order \( \delta m^{\text{sea}}/\Lambda \) where \( \Lambda \approx 10 m_s \). As we discuss below, \( g_{c,\alpha} \) can be estimated from perturbation theory and is again of order 1/10. We treat these coefficients as fit parameters in our analysis, with priors:

\[
g_\alpha = 0 \pm 0.1, \quad g_{a^2,\alpha} = 0 \pm 0.1, \quad g_{c,\alpha} = 0 \pm 0.1. \quad (A12)
\]

The rescaling factor \( \xi_\alpha \) is closely related to the dependence of the lattice spacing on the sea-quark masses used in the simulation. The lattice spacing is primarily a function of the bare coupling \( \alpha_{\text{lat}} \) used in the lattice action, but it also varies with the sea-quark masses, in our scheme, when the bare coupling is held constant. As discussed above, this is because of sea-mass dependence in the quantity used to define the lattice spacing, \( a/w_0 \) in our case. The relationship with \( \xi_\alpha \) can be understood by examining the \( \overline{\text{MS}} \) coupling at scale \( \mu = \pi/a \). There it is related to the bare coupling by a perturbative expansion,

\[
\alpha_{\overline{\text{MS}}}^{(\pi/a, \delta m^{\text{sea}})} = \alpha_{\overline{\text{MS}}}^{(\xi_\alpha \pi/a)} \\
= \alpha_{\text{lat}} + \sum_{n=2}^{\infty} c_n^{\overline{\text{MS}}} \alpha_{\text{lat}}^n, \quad (A13)
\]

that is mass-independent up to corrections of \( O((a m_c)^2 \alpha_s) \), which are negligible in our analysis. This formula implies that \( \alpha_{\overline{\text{MS}}}^{(\xi_\alpha \pi/a)} \) is constant if \( \alpha_{\text{lat}} \) is, and therefore that \( \xi_\alpha / a \) must be constant as well. Consequently the lattice spacing must vary with \( \delta m^{\text{sea}} \) like

\[
a(\delta m^{\text{sea}}) \approx \xi_\alpha \ a_{\text{phys}} \quad \text{(A14)}
\]

if the bare coupling is held constant, where \( a_{\text{phys}} \) is the lattice spacing when the sea-quark masses are tuned to their physical values — that is, \( a_{\text{phys}} = a(\delta m^{\text{sea}} = 0) \).

We use this variation in the lattice spacing to read off the parameters in \( \xi_\alpha \). Our simulation results fall into four groups of gluon ensembles, with lattice spacings around 0.15 fm, 0.12 fm, 0.09 fm and 0.06 fm. Each group corresponds to a single value of the bare lattice coupling \( \alpha_{\text{lat}} \), and several different values of light sea-quark mass. Within a single group, then, the values we obtain for \( a/w_0 \) from our simulations should vary as

\[
\frac{(a/w_0)_{\text{sim}}}{(a/w_0)_{\text{phys}}} = \xi_\alpha \times \frac{(a/w_0)_{\text{phys}}}{(a/w_0)_{\text{phys}}}, \quad \text{(A15)}
\]

where the parameters \( g_{a^2}, g_{a^2,\alpha} \) and \( g_{c,\alpha} \) in \( \xi_\alpha \) (Eq. A9) are the same for all four groups of data.

We fit our simulation results for \( a/w_0 \), simultaneously for all four groups, as functions of \( g_\alpha, g_{a^2,\alpha} \) and \( g_{c,\alpha} \). We also treat the value of \( (a/w_0)_{\text{phys}} \) for each group as a fit parameter. The resulting fit is shown in Fig. 8 where we plot

\[
\frac{(a/w_0)_{\text{sim}}}{(a/w_0)_{\text{phys}}} \quad \text{versus} \quad \delta m^{\text{sea}}/m_s.
\]

The fit is excellent, and shows that \( g_\alpha = 0.082(8) \). Our fit is not very sensitive to \( g_{a^2,\alpha} \) and \( g_{c,\alpha} \) — their impact on \( \xi_\alpha \) is too small — and gives results for these that are essentially the same as the prior values.

![FIG. 8. The ratio of the simulation lattice spacing with detuned sea-quark masses to the lattice spacing with physical sea-quark masses as a function of the light-quark mass detuning (in units of the s quark mass). Results are shown for four different sets of data, each corresponding to a different bare lattice coupling. The approximate lattice spacings for these sets are: 0.15 fm (red points), 0.12 fm (cyan), 0.09 fm (green), and 0.06 fm (blue). The dashed line and gray band show the mean and standard deviation of our best fit to these data. The fit has a \( \chi^2 \) per degree of freedom of 0.23 for 9 degrees of freedom (p-value of 0.99).](image-url)
3. \( m_h(\mu, \delta m_{\text{sea}}) \) and \( m_{0h}(\delta m_{\text{sea}}) \)

The evolution equations for the heavy quark’s \( \overline{\text{MS}} \) mass are unchanged by sea-mass detunings:

\[
\frac{d \log(m_h(\mu, \delta m_{\text{sea}}))}{d \log \mu^2} = \gamma_m(\alpha_{\text{MS}}(\mu, \delta m_{\text{sea}}))
\]

(A16)

Consequently any sea-mass dependence must enter through rescalings:

\[
m_h(\mu, \delta m_{\text{sea}}) = \xi_m m_h(\xi_\alpha \mu) \]

(A17)

where \( \xi_\alpha \) is defined above (Eq. (A9)), \( \xi_m \) is independent of \( \mu \), and

\[
m_h(\mu) \equiv m_h(\mu, \delta m_{\text{sea}} = 0)
\]

(A18)

is the \( \overline{\text{MS}} \) mass for physical sea-quark masses. We parameterize \( \xi_m \) similarly to \( \xi_\alpha \) but allowing for the coefficients to depend upon the heavy-quark mass:

\[
\xi_m = 1 + \frac{g_m}{(m_{\eta_s}/m_\eta)^\zeta} \frac{\delta m_{\text{sea}}}{m_a} + \frac{g_{a^2} m}{(m_{\eta_s}/m_\eta)^\zeta} \frac{\delta m_{\text{sea}}}{m_a} \left( \frac{m_a}{\pi/a} \right)^2 + \cdots
\]

(A19)

Again we expect \( g_m \) and \( g_{a^2} m \) to be of order 1/10, and we treat them as fit parameters with priors:

\[
g_m = 0 \pm 0.1, \quad g_{a^2} m = 0 \pm 0.1.
\]

We parameterize the dependence on heavy-quark mass with the factors \( (m_{\eta_s}/m_\eta)^\zeta \) where \( \zeta \) is a fit parameter with prior:

\[
\zeta = 0 \pm 1.
\]

(A21)

The sea-mass dependence in \( \xi_m \) comes from the quantity used to tune the heavy-quark mass in simulations. We tune these masses to give the correct physical mass for \( \eta_s \) — that is, the mass obtained when the sea-quark masses are tuned to their physical values and the lattice spacing is set to zero. This means that any sea-mass dependence in \( m_{\eta_s} \) is pushed into the rescaling factor \( \xi_m \) in Eq. (A17). The physical size of \( \eta_s \) mesons decreases as \( m_{\eta_s} \) increases, and this decreases the coupling with light sea-quarks. Thus we expect \( \xi > 0 \) in Eq. (A19); our fit finds \( \zeta = 0.3(1) \).

In principle, \( \xi_m \) should depend upon \( \delta m_{\text{sea}} \), as well as \( \delta m_{u_0} \). Perturbation theory, however, indicates that this dependence is negligible in our simulations. Thus we have omitted such terms from \( \xi_m \). We have verified that they are negligible by comparing fits that include \( \delta m_{\text{sea}} \) terms with the fit without them.

The rescaling factor \( \xi_m \) is closely related to the sea-mass dependence of the heavy quark’s bare mass, in much the same way \( \xi_\alpha \) is related to the lattice spacing. The bare mass \( m_{0h} \) is proportional to the \( \overline{\text{MS}} \) mass evaluated at \( \mu = \pi/a \):

\[
m_{0h} \propto m_h(\pi/a, \delta m_{\text{sea}})
\]

\[
\propto \xi_m m_h(\xi_\alpha \pi/a).
\]

(A22)

![Figure 9](image-url)

**FIG. 9.** The ratio of the bare \( c \) mass in lattice units used in the simulations to the bare mass with physical sea-quark masses as a function of the light-quark mass detuning (in units of the \( s \) quark mass). Results are shown for four different sets of data, each corresponding to a different bare lattice coupling. The approximate lattice spacings for these sets are: 0.15 fm (red points), 0.12 fm (cyan), 0.09 fm (green), and 0.06 fm (blue). The dashed line and gray band show the mean and standard deviation of our best fit to these data. The fit has a \( \chi^2 \) per degree of freedom of 0.15 for 9 degrees of freedom (p-value of 1.0).

Since \( \xi_\alpha/a \) is sea-mass independent, we see that \( m_{h0} \) is proportional to \( \xi_m \),

\[
m_{0h}(\delta m_{\text{sea}}) = \xi_m m_{0h}^{\text{phys}},
\]

(A23)

when the sea-quark masses are varied while holding the bare coupling fixed.

This variation can be used to determine the parameters in \( \xi_m \), again in analogy to the previous section. As discussed in the previous section, our ensembles fall into four groups each corresponding to a different value of the bare coupling constant \( \alpha_{\text{lat}} \). The masses \( m_{0h}^{\text{tuned}} \) for each ensemble in Table III are tuned to give the physical \( \eta_s \) mass for that ensemble. Therefore, within each group of ensembles, we expect

\[
am_{0c}^{\text{tuned}} = \xi_\alpha \xi_m \times (am_{0c})_{\text{phys}}
\]

(A24)

where \( (am_{0c})_{\text{phys}} \) is the value for properly tuned sea-quark masses.

We fit our simulation results for \( am_{0c}^{\text{tuned}} \) as functions of \( g_m, g_{a^2} m, g_{a^2}, a_0, g_{a^2}, a_0 \), and \( g_{a^2} a_0 \). We use best-fit values from the fit in the previous section as priors for the last three of these fit parameters. The values of \( (am_{0c})_{\text{phys}} \) for the different groups of ensembles are also fit parameters.

The resulting fit is shown in Fig. 9 where we plot \( am_{0c}^{\text{tuned}}/(am_{0c})_{\text{phys}} \) as a function of \( \delta m_{\text{sea}}/m_s \). The fit is excellent and shows that \( g_m = 0.035(5) \), while \( g_{a^2} m \) is essentially unchanged from its prior value (because our data are not sufficiently accurate).
4. c Quarks and Decoupling

Heavy quarks decouple from low-energy physics, and therefore variations in $\delta m_c^{\text{sea}}$ should have no impact on physics (like $w_0$) that probes momentum scales smaller than $m_c$. We can, however, introduce (apparent) violations of the decoupling theorem through the scheme used to set the lattice spacing. In particular, decoupling is violated by any scheme that holds the lattice spacing fixed (together with the bare coupling $\alpha_s^{(n_f)}$) as $\delta m_c^{\text{sea}}$ is varied. On the contrary, decoupling is preserved by schemes that hold a low-energy ($< 2m_c$) quantity like $w_0$ fixed, instead of the lattice spacing $\Lambda$.

The difference between these schemes arises because the running of the QCD coupling is modified in a detuned theory for scales between $m_c^{\text{sea}}$ and $m_c^{\text{sea}} + \delta m_c^{\text{sea}}$, resulting in a mismatch between low and high energy values of the coupling. Physics below $m_c$ is determined by the $n_f = 3$ coupling constant, which, by decoupling, should be independent of $\delta m_c^{\text{sea}}$.

To see how this works, we examine lowest-order perturbation theory where

$$\alpha_s^{(n_f)}(\mu) = \frac{2\pi}{\beta(n_f) \log(\mu/\Lambda^{(n_f)})}$$ (A25)

with $\beta(n_f) \equiv 11 - 2n_f/3$, and

$$\alpha_s^{(3)}(\mu) = \alpha_s^{(4)}(\mu, \delta m_c^{\text{sea}})$$ (A26)

at $\mu = m_c + \delta m_c^{\text{sea}}$. Here $\Lambda^{(3)}$ must be independent of $\delta m_c^{\text{sea}}$, by decoupling, while $\Lambda^{(4)}$ must vary with $\delta m_c^{\text{sea}}$ to cancel the effect of the shift in the match point $\mu = m_c + \delta m_c^{\text{sea}}$. It is straightforward to show that

$$\Lambda^{(4)}(\delta m_c^{\text{sea}}) \approx m_c \left( \frac{\Lambda^{(3)}}{m_c} \right)^{\beta(3)/\beta(4)} \left( 1 - 2 \frac{\delta m_c^{\text{sea}}}{25 m_c} \right)$$

$$\approx \Lambda^{(\text{phys})} \times \left( 1 - 2 \frac{\delta m_c^{\text{sea}}}{25 m_c} \right)$$ (A27)

where $\Lambda^{(\text{phys})}$ is the value for physical sea-quark masses. Thus the decoupling theorem requires that

$$\alpha_s^{(4)}(\mu, \delta m_c^{\text{sea}}) = \alpha_s^{(4)}(\mu) \times \left( 1 + 2 \frac{\delta m_c^{\text{sea}}}{25 m_c} \right)$$ (A28)

By comparing with Eqs. (A7) and (A9), we see that

$$g_{c,\alpha} = 2 \frac{\delta m_c^{\text{sea}}}{25} + O(\alpha_s)$$ (A29)

and, therefore, that the lattice spacing varies with $\delta m_c^{\text{sea}}$ (Eq. (A14)).

There is an analogous effect in the heavy-quark mass, but the mass dependence in $\delta m$ is suppressed by $\alpha_s^2$ and so is negligible in our analysis.

This analysis shows that a constant lattice spacing is incompatible with the decoupling theorem. The scheme we use avoids this problem by allowing the lattice spacing to vary with $\delta m_c^{\text{sea}}$, while holding the value of $w_0$ constant (as required by the decoupling theorem applied to $w_0$ itself). The violation of the decoupling theorem in the former case is only apparent; results from all schemes should agree when the sea-quark masses are tuned to their physical values.
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