

Update of $|V_{cb}|$ from the $\bar{B} \rightarrow D^* \ell \bar{\nu}$ form factor at zero recoil with three-flavor lattice QCD

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Abstract

We compute the zero-recoil form factor for the semileptonic decay $\bar{B}^0 \rightarrow D^{*+}\ell^-\bar{\nu}$ (and modes related by isospin and charge conjugation) using lattice QCD with three flavors of sea quarks. We use an improved staggered action for the light valence and sea quarks (the MILC asqtad configurations), and the Fermilab action for the heavy quarks. Our calculations incorporate higher statistics, finer lattice spacings, and lighter quark masses than our 2008 work. As a byproduct of tuning the new data set, we obtain the D_s and B_s hyperfine splittings with few-MeV accuracy. For the zero-recoil form factor, we obtain $\mathcal{F}(1) = 0.906(4)(12)$, where the first error is statistical and the second is the sum in quadrature of all systematic errors. With the latest HFAG average of experimental results and a cautious treatment of QED effects, we find $|V_{cb}| = (39.04 \pm 0.49_{\text{expt}} \pm 0.53_{\text{QCD}} \pm 0.19_{\text{QED}}) \times 10^{-3}$. The QCD error is now commensurate with the experimental error.

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I. INTRODUCTION

The Cabibbo-Kobayashi-Maskawa (CKM) matrix element $|V_{cb}|$ is one of the fundamental parameters of the Standard Model (SM). Together with $|V_{us}|$, $|V_{ub}|$, and $\arg V_{ub}^*$, it allows for a full SM determination of flavor and CP violation via processes that proceed at the tree level of the electroweak interaction. In the case of $|V_{cb}|$, one requires a measurement of the differential rate of B mesons decaying semileptonically to a charmed final state. The hadronic part of the final state can be exclusive—*e.g.*, a D^* or D meson—or inclusive.

The 2012 edition of the Review of Particle Physics by the Particle Data Group (PDG) [1] notes that the exclusive and inclusive values of $|V_{cb}|$ are marginally consistent with each other. Furthermore, global fits to a comprehensive range of flavor- and CP -violating observables tend to prefer the inclusive value [2–4]: when direct information on $|V_{cb}|$ is omitted from the fit, one of the outputs of the fit is a value of $|V_{cb}|$ that agrees better with the inclusive than the exclusive value. One should bear in mind that some tension in the global fits to the whole CKM paradigm has been seen [5]. A full discussion of the possible resolutions of the discrepancy lies beyond the scope of this article. We conclude merely that it is important and timely to revisit the theoretical and experimental ingredients of both determinations.

In this paper, we improve the lattice-QCD calculation [6–8] of the zero-recoil form factor for the exclusive decay $\bar{B} \rightarrow D^* \ell \bar{\nu}$ (and isopin-partner and charge-conjugate modes). Our analysis strategy is very similar to our previous work [7], but the lattice-QCD data set is much more extensive, with higher statistics on all ensembles, smaller lattice spacings (as small as $a \approx 0.045$ fm) and light-quark masses as small as $\hat{m}' = m_s/20$ (at lattice spacing $a \approx 0.09$ fm). Figure 1 provides a simple overview of the new and old data sets; further details are given in Sec. II. Our preliminary status report [8] encompassed the higher statistics but not yet four of the ensembles in the lower left-hand corner of Fig. 1.

With this work, we improve the precision of $|V_{cb}|$ as determined from exclusive decays

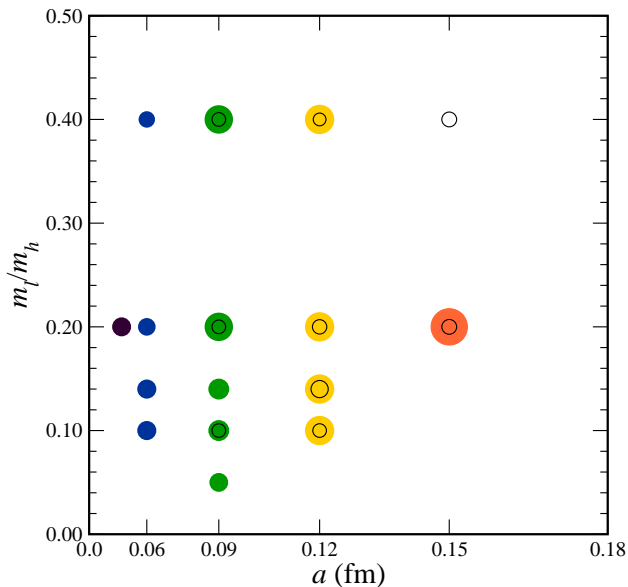


FIG. 1. (color online) Range of lattice spacings and light-quark masses used here (colored or gray discs) and in Ref. [7] (black circles). The area is proportional to the size of the ensemble. The lattice spacings are $a \approx 0.15, 0.12, 0.09, 0.06$, and 0.045 fm. Reference [8] did not yet include the ensembles with $(a, \hat{m}'/m_s) = (0.045 \text{ fm}, 0.20), (0.06 \text{ fm}, 0.14), (0.06 \text{ fm}, 0.10)$, and $(0.09 \text{ fm}, 0.05)$.

to that claimed for the determination from inclusive decays: 2%. Moreover, we reduce the QCD uncertainty on $|V_{cb}|$ to the same level as the experimental uncertainty. Because $|V_{cb}|$ normalizes the unitarity triangle, it appears throughout flavor physics. For example, the SM expressions for ε_K and for the branching ratios of the golden modes $K^+ \rightarrow \pi^+ \nu \bar{\nu}$ and $K_L \rightarrow \pi^0 \nu \bar{\nu}$ all contain $|V_{cb}|^4$. Therefore, further improvements—beyond what is achieved here—are warranted, particularly during the course of the Belle II experiment [9].

The amplitude for $B \rightarrow D^*$ semileptonic decay is expressed in terms of form factors,

$$\frac{\langle D^*(p_{D^*}, \epsilon^{(\alpha)}) | \mathcal{A}^\mu | B(p_B) \rangle}{\sqrt{2M_{D^*}} \sqrt{2M_B}} = \frac{i}{2} \epsilon_\nu^{(\alpha)*} [g^{\mu\nu} (1+w) h_{A_1}(w) - v_B^\nu (v_B^\mu h_{A_2}(w) + v_{D^*}^\mu h_{A_3}(w))], \quad (1.1)$$

$$\frac{\langle D^*(p_{D^*}, \epsilon^{(\alpha)}) | \mathcal{V}^\mu | B(p_B) \rangle}{\sqrt{2M_{D^*}} \sqrt{2M_B}} = \frac{1}{2} \varepsilon^{\mu\nu\rho\sigma} \epsilon_\nu^{(\alpha)*} v_B^\rho v_{D^*}^\sigma h_V(w), \quad (1.2)$$

where \mathcal{A}^μ and \mathcal{V}^μ are the (continuum QCD) $b \rightarrow c$ electroweak currents, $v_B^\mu = p_B^\mu/M_B$, $v_{D^*}^\mu = p_{D^*}^\mu/M_{D^*}$, the velocity transfer $w = v_B \cdot v_{D^*}$, and $\epsilon^{(\alpha)}$ is the polarization vector of the D^* meson. In the SM, the differential rate for $B^- \rightarrow D^{0*} \ell^- \bar{\nu}$ (and the charge-conjugate mode) is given by

$$\frac{d\Gamma}{dw} = \frac{G_F^2 M_{D^*}^3}{4\pi^3} (M_B - M_{D^*})^2 (w^2 - 1)^{1/2} |\eta_{\text{EW}}|^2 |V_{cb}|^2 \chi(w) |\mathcal{F}(w)|^2, \quad (1.3)$$

where η_{EW} provides a structure-independent electroweak correction from next-to-leading-order box diagrams, in which a photon or Z boson is exchanged along with the W boson [10]. (See Sec. VIII for details.) The rate for $\bar{B}^0 \rightarrow D^{+*} \ell^- \bar{\nu}$ (and charge conjugate) is the same as Eq. (1.3) but with an additional factor on the right-hand side $(1 + \pi\alpha)$ [11, 12], which accounts for the Coulomb attraction of the final-state charged particles.

The notation $\chi(w) |\mathcal{F}(w)|^2$ is conventional, motivated by the heavy-quark limit. In the zero-recoil limit, $w \rightarrow 1$, one has $\chi(w) \rightarrow 1$, and only one form factor survives:

$$\mathcal{F}(1) = h_{A_1}(1). \quad (1.4)$$

From Eq. (1.1), one sees that the needed matrix element is $\langle D^* | \epsilon^{(\alpha)} \cdot \mathcal{A} | B \rangle$ with initial and final states both at rest.

For nonvanishing lepton mass m_ℓ , the rate is multiplied by $(1 - m_\ell^2/q^2)^2$, and the expressions for $\chi(w)$ and $|\mathcal{F}(w)|^2$ receive corrections proportional to m_ℓ^2/q^2 [13]. At zero recoil, these corrections reduce to an additional factor $(1 + m_\ell^2/q_{\text{max}}^2)$ on the right-hand side of Eq. (1.4). Except for $\ell = \tau$, lepton mass effects are not important even at the current level of accuracy.

Because precision is so crucial, the lattice-QCD calculation must be set up in a way that ensures considerable cancellation of all sources of uncertainty. The pioneering work of Hashimoto *et al.* [6, 14] introduced several double ratios to this end. Here, we follow Ref. [7] and use a single, direct double ratio

$$\mathcal{R}_{A_1} = \frac{\langle D^* | \bar{c} \gamma^j \gamma^5 b | \bar{B} \rangle \langle \bar{B} | \bar{b} \gamma^j \gamma^5 c | D^* \rangle}{\langle D^* | \bar{c} \gamma^4 c | D^* \rangle \langle \bar{B} | \bar{b} \gamma^4 b | \bar{B} \rangle} = |h_{A_1}(1)|^2 \quad (1.5)$$

with all states at rest and the polarization of the D^* aligned with j . In the continuum, the denominator of Eq. (1.5) is unity, by the definition of the flavor quantum numbers. On the lattice, however, it normalizes the flavor numbers *and* cancels statistical fluctuations. The

main uncertainties stem, then, from the chiral extrapolation (the light-quark masses in our data exceed the up and down masses) and discretization and matching errors. In particular, we show how the discretization errors of the analogous ratio of lattice-QCD correlation functions are reduced by use of the ratio.

The rest of this paper is organized as follows. Section II describes the details of the lattice-QCD calculation. We discuss the lattice implementation of Eq. (1.5), the details of the numerical data, and the general structure of the computed correlation functions. Section III describes our fits to a ratio of correlation functions. Section IV discusses perturbative matching. Section V summarizes the tuning of the bottom- and charm-quark masses and presents results for the D_s and B_s hyperfine splittings. Our extrapolation to the continuum limit and physical light-quark mass is described in Sec. VI. Section VII gives full details of our systematic error analysis. Section VIII provides a discussion of electroweak and electromagnetic effects, which, though separate from our QCD calculation, are needed to obtain $|V_{cb}|$. Section IX concludes with final results for $h_{A_1}(1)$ and $|V_{cb}|$. The appendices contain additional material, including the formulas used for the chiral extrapolation (Appendix A), an estimate of heavy-quark discretization errors (Appendix B), and a thorough discussion of our procedure for tuning the bottom- and charm-quark masses (Appendix C), which also yields the hyperfine splitting.

II. LATTICE SETUP

In this section we discuss the ingredients of our lattice-QCD calculation. We outline first the generation of ensembles of lattice gauge fields, and then the procedures for computing the three-point correlation functions needed to obtain the double ratio R_{A_1} , which is the lattice correlation-function analog of \mathcal{R}_{A_1} .

A. Simulation parameters

We use the MILC ensembles [15] of lattice gauge fields listed in Table I. The ensembles were generated with a Symanzik-improved gauge action [16–19] and 2+1 flavors of sea quarks. The couplings in the gauge action include the one-loop effects of gluons [20] but not of sea quarks [21]; the latter were not yet available when the gauge-field generation began [22]. The sea-quark action is the order a^2 , tadpole-improved (asqtad) action [23–27] for staggered quarks [28, 29]. To reduce the species content from the four that come with staggered fermions, the light quarks (strange quark) are simulated with the square root (fourth root) of the determinant [30]. At nonzero lattice spacing this procedure introduces small violations of unitarity [31–34] and locality [35]. Considerable numerical and theoretical evidence suggests that these effects go away in the continuum limit, so that the procedure yields QCD [32, 36–44].

As one can see from Table I, some ensembles contain ~ 2000 independent gauge fields, others ~ 600 –1000. To increase statistics, we re-use each field four times (for $a \approx 0.15$ fm, 24 times) by computing quark propagators that are evenly spaced in the time direction with a spatial source origin that is chosen at random from one configuration to the next.

We also use the asqtad action for the light valence (spectator) quark. In this paper, we denote the physical quark masses by m_u , m_d , $\hat{m} = \frac{1}{2}(m_u + m_d)$, and m_s ; the variable spectator mass by m_x ; and the sea-quark masses \hat{m}' and m'_s , which are fixed within each

TABLE I. Parameters of the lattice gauge fields. The columns from left to right are the approximate lattice spacing in fm, the sea-quark masses $a\hat{m}'/am'_s$, the linear spatial dimension of the lattice ensemble in fm, the dimensionless factor $m_\pi L$ (with m_π from the Goldstone pion), the gauge coupling, the dimensions of the lattice in lattice units, the number of sources and configurations in each ensemble, and the tadpole improvement factor u_0 (obtained from the average plaquette).

a (fm)	$a\hat{m}'/am'_s$	L (fm)	$m_\pi L$	$10/g^2$	Volume	Sources×Configs	u_0
0.15	0.0097/0.0484	2.4	3.9	6.572	$16^3 \times 48$	24×628	0.8604
0.12	0.02/0.05	2.4	6.2	6.79	$20^3 \times 64$	4×2052	0.8688
0.12	0.01/0.05	2.4	4.5	6.76	$20^3 \times 64$	4×2256	0.8677
0.12	0.007/0.05	2.4	3.8	6.76	$20^3 \times 64$	4×2108	0.8678
0.12	0.005/0.05	2.9	3.8	6.76	$24^3 \times 64$	4×2096	0.8678
0.09	0.0124/0.031	2.4	5.8	7.11	$28^3 \times 96$	4×1992	0.8788
0.09	0.0062/0.031	2.4	4.1	7.09	$28^3 \times 96$	4×1928	0.8782
0.09	0.00465/0.031	2.7	4.1	7.085	$32^3 \times 96$	4×984	0.8781
0.09	0.0031/0.031	3.4	4.2	7.08	$40^3 \times 96$	4×1012	0.8779
0.09	0.00155/0.031	5.5	4.8	7.075	$64^3 \times 96$	4×788	0.877805
0.06	0.0072/0.018	2.9	6.3	7.48	$48^3 \times 144$	4×576	0.8881
0.06	0.0036/0.018	2.9	4.5	7.47	$48^3 \times 144$	4×672	0.88788
0.06	0.0025/0.018	3.4	4.4	7.465	$56^3 \times 144$	4×800	0.88776
0.06	0.0018/0.018	3.8	4.3	7.46	$64^3 \times 144$	4×824	0.88764
0.045	0.0028/0.014	2.9	4.6	7.81	$64^3 \times 192$	4×800	0.89511

ensemble. The bare spectator masses am_x are listed in Table II. In every case, we compute light-quark propagators with the valence mass equal to the light mass, $am_x = a\hat{m}'$, and, in several cases, we also compute a partially quenched propagator with $am_x = 0.4am'_s$.

For the heavy b and c quarks we use Wilson fermions [45] with the Sheikholeslami-Wohlert (SW) action [46], adjusting the parameters in the action according to the Fermilab method [47]. Table II also lists the parameters of the heavy-quark action: the hopping parameter κ (for each quark) and the clover coefficient of the SW action. We use κ'_b and κ'_c to denote the values used in the computations, reserving κ_b and κ_c for those that reproduce the B_s and D_s meson masses most accurately. We set c_{SW} to the value from tree-level tadpole-improved perturbation theory, $c_{\text{SW}} = u_0^{-3}$, with u_0 from Table I. Table III gives the values of κ_{crit} where the quark mass vanishes for the SW action on each of our ensembles. These values were determined using the methods discussed in Ref. [48]; note that κ_{crit} is only needed in the present work to fix the improvement coefficients that correct the lattice currents described below.

The relative lattice spacing is determined by calculating r_1/a on each ensemble, where r_1 is related to the heavy-quark potential and is defined such that the force between static quarks, $r_1^2 F(r_1) = 1.0$ [49, 50]. A mass-independent procedure is used to set r_1/a . This procedure takes the measured values $r_1(\hat{m}', m'_s, \beta)/a$ and constructs a smooth interpolation/extrapolation, which we use to replace the measured values with $r_1(\hat{m}, m_s, \beta)/a$, evaluated now at the physical masses \hat{m} , m_s . Table III lists r_1/a values for each of the ensembles that results from fitting the calculated r_1/a to the smooth function and extrapolating/interpolating to physical masses. The absolute lattice spacing requires a physical

TABLE II. Valence-quark parameters used in the simulations. The (approximate) lattice spacings a and the sea-quark masses $a\hat{m}'/am'_s$ (first two columns) identify the ensemble. Here, am_x denotes the bare masses for the light spectator quarks, c_{SW} and κ denote the parameters in the SW action, and d_1 the rotation parameter in the current. The primes on κ and d_1 distinguishes the simulation from the physical values.

a (fm)	$a\hat{m}'/am'_s$	am_x	c_{SW}	κ'_b	d'_{1b}	κ'_c	d'_{1c}
0.15	0.0097/0.0484	0.0097, 0.0194	1.567	0.0781	0.08354	0.1218	0.08825
0.12	0.02/0.05	0.02	1.525	0.0918	0.09439	0.1259	0.07539
0.12	0.01/0.05	0.01, 0.02	1.531	0.0901	0.09334	0.1254	0.07724
0.12	0.007/0.05	0.007, 0.02	1.530	0.0901	0.09332	0.1254	0.07731
0.12	0.005/0.05	0.005, 0.02	1.530	0.0901	0.09332	0.1254	0.07733
0.09	0.0124/0.031	0.0124	1.473	0.0982	0.09681	0.1277	0.06420
0.09	0.0062/0.031	0.0062, 0.0124	1.476	0.0979	0.09677	0.1276	0.06482
0.09	0.00465/0.031	0.00465	1.477	0.0977	0.09671	0.1275	0.06523
0.09	0.0031/0.031	0.0031, 0.0124	1.478	0.0976	0.09669	0.1275	0.06537
0.09	0.00155/0.031	0.00155	1.4784	0.0976	0.09669	0.1275	0.06543
0.06	0.0072/0.018	0.0072	1.4276	0.1048	0.09636	0.1295	0.05078
0.06	0.0036/0.018	0.0036, 0.0072	1.4287	0.1052	0.09631	0.1296	0.05055
0.06	0.0025/0.018	0.0025	1.4293	0.1052	0.09633	0.1296	0.05070
0.06	0.0018/0.018	0.0018	1.4298	0.1052	0.09635	0.1296	0.05076
0.045	0.0028/0.014	0.0028	1.3943	0.1143	0.08864	0.1310	0.03842

quantity to set the scale. We take the absolute lattice spacing to be $r_1 = 0.3117(22)$ fm from the MILC determination of f_π . The value used is explained and justified in Ref. [51].

We have to adjust the light-quark bare masses and the heavy-quark hopping parameters to their physical values *a posteriori*. The adjustment of the light-quark masses is carried out in the chiral extrapolation, discussed in Sec. VI. For the heavy quarks, we have chosen κ'_b and κ'_c in Table II close to the physical value based on an initial set of runs that studied a range of κ but computed only the two-point functions for heavy-strange meson masses. After the full runs, including three-point functions, we re-analyzed the two-point functions to determine more precise κ values, as discussed in detail in Appendix C. Using information on the κ dependence, we can then fine-tune our result.

B. $B \rightarrow D^*$ correlation functions

To obtain the matrix elements in Eq. (1.5), we compute the correlation functions

$$C^{B \rightarrow D^*}(t_s, t_f) = \sum_{\mathbf{x}, \mathbf{y}} \langle \mathcal{O}_{D^*}(\mathbf{x}, t_f) A_{cb}^j(\mathbf{y}, t_s) \mathcal{O}_B^\dagger(\mathbf{0}, 0) \rangle, \quad (2.1)$$

$$C^{B \rightarrow B}(t_s, t_f) = \sum_{\mathbf{x}, \mathbf{y}} \langle \mathcal{O}_B(\mathbf{x}, t_f) V_{bb}^4(\mathbf{y}, t_s) \mathcal{O}_B^\dagger(\mathbf{0}, 0) \rangle, \quad (2.2)$$

and similarly $C^{D^* \rightarrow B}$ and $C^{D^* \rightarrow D^*}$. Here, \mathcal{O}_B and \mathcal{O}_{D^*} are lattice operators with quantum numbers needed to annihilate B and D^* mesons, in the case of D^* with polarization in the

TABLE III. Derived parameters that enter the simulations. The (approximate) lattice spacings a and the sea-quark masses $a\hat{m}'/am'_s$ (first two columns) identify the ensemble. Values for r_1/a are given in column three, and κ_{crit} values for the SW action evaluated on our ensembles are given in column four. For r_1/a , statistical errors are 0.1 to 0.3%, and the systematic errors are comparable. For κ_{crit} the errors are a few in the last quoted digit.

a (fm)	$a\hat{m}'/am'_s$	r_1/a	κ_{crit}
0.15	0.0097/0.0484	2.2215	0.142432
0.12	0.02/0.05	2.8211	0.14073
0.12	0.01/0.05	2.7386	0.14091
0.12	0.007/0.05	2.7386	0.14095
0.12	0.005/0.05	2.7386	0.14096
0.09	0.0124/0.031	3.8577	0.139052
0.09	0.0062/0.031	3.7887	0.139119
0.09	0.00465/0.031	3.7716	0.139134
0.09	0.0031/0.031	3.7546	0.139173
0.09	0.00155/0.031	3.7376	0.13919
0.06	0.0072/0.018	5.3991	0.137582
0.06	0.0036/0.018	5.3531	0.137632
0.06	0.0025/0.018	5.3302	0.137667
0.06	0.0018/0.018	5.3073	0.137678
0.045	0.0028/0.014	7.2082	0.13664

j direction; V_{cb}^μ and A_{cb}^μ are lattice currents for $b \rightarrow c$ transitions.

We form the interpolating operators from a staggered fermion field χ and heavy-quark field ψ in the SW action:

$$\mathcal{O}_{D_j^*}(\mathbf{x}, t) = \sum_{\mathbf{w}} \bar{\chi}(\mathbf{x}, t) \Omega^\dagger(\mathbf{x}, t) i\gamma_j S(\mathbf{x}, \mathbf{w}) \psi_c(\mathbf{w}, t), \quad (2.3)$$

$$\mathcal{O}_B^\dagger(\mathbf{x}, t) = \sum_{\mathbf{w}} \bar{\psi}_b(\mathbf{w}, t) S(\mathbf{w}, \mathbf{x}) \gamma_5 \Omega(\mathbf{x}, t) \chi(\mathbf{x}, t), \quad (2.4)$$

$$\Omega(x) = \gamma_1^{x_1/a} \gamma_2^{x_2/a} \gamma_3^{x_3/a} \gamma_4^{x_4/a}, \quad [x = (\mathbf{x}, t)], \quad (2.5)$$

where $S(\mathbf{x}, \mathbf{y})$ is a spatial smearing function. The free Dirac index on Ω can be interpreted as a taste index (in which case we average over taste) [42], or one can promote χ to a four-component field [52], which leads to the same results for the correlation functions of bilinear operators.

We employ two smearing functions. One is the local $S(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y})$. The other is the ground-state 1S wavefunction of the Richardson potential. See Ref. [51] for details.

We define the lattice vector and axial-vector currents to be

$$V_{hh}^\mu = \bar{\Psi}_h \gamma^\mu \Psi_h, \quad (2.6)$$

$$A_{cb}^\mu = \bar{\Psi}_c \gamma^\mu \gamma^5 \Psi_b, \quad (2.7)$$

where $h = b, c$ are flavor indices. The fermion field Ψ includes a correction factor to reduce discretization effects [47],

$$\Psi_h = (1 + d_1 \boldsymbol{\gamma} \cdot \mathbf{D}_{\text{lat}}) \psi_h, \quad (2.8)$$

where D_{lat}^μ is a nearest-neighbor covariant difference operator. Its coefficient d_1 is set to its value in tree-level tadpole-improved perturbation theory, where it does not depend on the other quark in the current. The matrix elements of the lattice currents satisfy (\doteq means “has the same matrix elements as”) [53, 54]

$$Z_{J_{cb}^\mu} J^\mu \doteq \mathcal{J}^\mu + \mathcal{O}(\alpha_s^{1+\ell_Z}, \alpha_s^{1+\ell_d} a, a^2), \quad (2.9)$$

where \mathcal{J}^μ is the continuum current corresponding to the lattice current J^μ and the matching factors $Z_{J_{cb}^\mu}$ are defined such that Eq. (2.9) holds. In practice, $Z_{J_{cb}^\mu}$ can be determined only approximately, via either perturbative or nonperturbative methods. Thus, $\ell_{Z \text{ or } d} = 0$ for tree-level matching of Z or d_1 , $\ell_{Z \text{ or } d} = 1$ for one-loop matching, etc. Nonperturbative matching schemes could be set up, which would remove all powers of α_s . Here we implicitly use nonperturbative matching for flavor-diagonal $Z_{V_{hh}^4}$, one-loop matching for suitable ratios of Z_J factors (see below), and tree-level matching for d_1 . Higher-loop and nonperturbative calculations, except for $Z_{V_{hh}^4}$, are not available.

In the double ratio like Eq. (1.5) but with matrix elements of lattice currents, the following ratio of matching factors remains:

$$\rho_{A^i}^2 = \frac{Z_{A_{cb}^i} Z_{A_{bc}^i}}{Z_{V_{cc}^4} Z_{V_{bb}^4}}. \quad (2.10)$$

In this ratio, all corrections associated with wave-function renormalization cancel out, leaving only vertex diagrams. Each Z contains the difference between continuum and lattice vertex diagrams, and the ratio introduces further cancellations. It is not surprising, then, that one-loop calculations of ρ_{A^i} yield very small coefficients of α_s [54].

With the Fermilab method applied to the SW action, the Lagrangian also leads to discretization effects of order $\mathcal{O}(\alpha_s^{1+\ell_c} a, a^2)$, where ℓ_c counts, as above, the matching of the SW (clover) term. Again, one-loop matching is not completely available (see Ref. [55]), so we use tree-level matching. Table II lists the values of c_{SW} used in this work. Appendix B discusses the discretization effects in $h_{A_1}(1)$ (as extracted here) in detail.

For large enough time separations t_s and $t_f - t_s$, the correlation function

$$C^{B \rightarrow D^*}(t_s, t_f) = \mathcal{Z}_{D^*}^{1/2} \mathcal{Z}_B^{1/2} \frac{\langle D^* | A_{cb}^j | \bar{B} \rangle}{\sqrt{2M_{D^*}} \sqrt{2M_B}} e^{-M_B t_s} e^{-M_{D^*}(t_f - t_s)} + \dots, \quad (2.11)$$

where M_B and M_{D^*} are the masses of the B and D^* mesons and $\mathcal{Z}_H = |\langle 0 | \mathcal{O}_H | H \rangle|^2 / 2M_H$. The omitted terms from higher-mass states are discussed in Sec. III. The other correlation functions $C^{D^* \rightarrow B}$, $C^{B \rightarrow B}$, $C^{D^* \rightarrow D^*}$ have analogous large-time behavior. Therefore, the ratio of correlation functions

$$R(t_s, t_f) \equiv \frac{C^{B \rightarrow D^*}(t_s, t_f) C^{D^* \rightarrow B}(t_s, t_f)}{C^{D^* \rightarrow D^*}(t_s, t_f) C^{B \rightarrow B}(t_s, t_f)} \rightarrow R_{A_1}, \quad (2.12)$$

where

$$R_{A_1} = \frac{\langle D^* | A_{cb}^j | \bar{B} \rangle \langle \bar{B} | A_{bc}^j | D^* \rangle}{\langle D^* | V_{cc}^4 | D^* \rangle \langle \bar{B} | V_{bb}^4 | \bar{B} \rangle} = \left| \frac{h_{A_1}(1)}{\rho_{A^j}} \right|^2 + \dots, \quad (2.13)$$

is a lattice version of \mathcal{R}_{A_1} , up to the matching factor ρ_{A^j} and discretization errors. The analysis of $R(t_s, t_f)$ to extract R_{A_1} is discussed in Sec. III, the calculation of ρ_{A^j} is discussed

in Sec. IV, the light-quark discretization errors are analyzed in Sec. VI, and the heavy-quark discretization errors are derived in Appendix B.

Above we mentioned that we increase statistics by choosing four (24 at $a \approx 0.15$ fm) sources. This means we choose four (24) origins $(\mathbf{0}, 0)$ in Eqs. (2.1) and (2.2). We do so by picking at random four (24) equally separated timeslices for $t = 0$. On each timeslice, we choose a completely random point for $\mathbf{x} = \mathbf{0}$.

Starting at each origin $[(\mathbf{0}, 0)$ in Eqs. (2.1) and (2.2)], we construct the three-point correlation functions as follows. We compute the parent heavy-quark propagator from smeared $(\mathbf{0}, 0)$ to all points, in particular (\mathbf{y}, t_s) . We also compute the spectator staggered-quark propagator from $(\mathbf{0}, 0)$ to all points. At time t_f , we convolve this propagator with the Dirac matrix and smearing function of the sink, projecting onto a fixed momentum (here, $\mathbf{p} = \mathbf{0}$). This combination is used for a further inversion for the daughter heavy quark; this inversion yields a sequential propagator encoding the propagation of the spectator quark, a flavor change at the sink, and (reverse) propagation of the daughter quark back to the decay. This sequential propagator and the parent propagator are then inserted into the appropriate trace over color and Dirac indices.

III. ANALYSIS OF CORRELATION FUNCTIONS

To obtain R_{A_1} from $R(t_s, t_f)$ with sufficient accuracy, we have to treat the excited states [denoted by \dots in Eq. (2.11)] carefully. From the transfer-matrix formalism, one finds

$$C^{X \rightarrow Y}(t_s, t_f) = \sum_{r=0}^{\infty} \sum_{s=0}^{\infty} (-1)^{rt_s/a} (-1)^{s(t_f-t_s)/a} A_{sr} e^{-M_X^{(r)} t_s} e^{-M_Y^{(s)}(t_f-t_s)} \quad (3.1)$$

where even r and s label radial excitations of desired parity, and odd r and s label excitations of opposite parity. The appearance of the opposite-parity states and their oscillating time dependence are consequences of using staggered fermions for the spectator quark. The A_{rs} are transition matrix elements, multiplied by uninteresting factors. For the desired A_{00} , these factors cancel in R_{A_1} .

In practice, we can choose the time separations such that only the lowest-lying states of each parity make a significant contribution. As discussed in detail in Ref. [7], it is advantageous to smear over time in a way that suppresses the opposite-parity state, and define

$$\bar{R}(t_s, t_f) \equiv \frac{1}{2} R(t_s, t_f) + \frac{1}{4} R(t_s, t_f + 1) + \frac{1}{4} R(t_s + 1, t_f + 1), \quad (3.2)$$

which is very close to R_{A_1} , with small time-dependent effects that one can disentangle via a fit to the t_s dependence.

The average in Eq. (3.2) is designed to suppress the contribution from oscillating states that changes sign only when the total source-sink separation is varied (the ‘‘same-sign’’ oscillating-state contributions). The double ratio, including the leading effects of the wrong-parity states, is

$$\bar{R}_{A_1}(t_s, t_f) = \frac{A_{00}^{B \rightarrow D^*} A_{00}^{D \rightarrow B^*}}{A_{00}^{D \rightarrow D^*} A_{00}^{B \rightarrow B^*}} \left[1 + \bar{c}^{B \rightarrow D^*}(t_s, t_f) + \bar{c}^{D \rightarrow B^*}(t_s, t_f) - \bar{c}^{D \rightarrow D^*}(t_s, t_f) - \bar{c}^{B \rightarrow B^*}(t_s, t_f) + \dots \right], \quad (3.3)$$

where the function $\bar{c}^{X \rightarrow Y}$ contains the oscillating-state contributions, and is given by

$$\begin{aligned} \bar{c}^{X \rightarrow Y}(t_s, t_f) \equiv & \frac{A_{01}^{X \rightarrow Y}}{A_{00}^{X \rightarrow Y}} (-1)^{t_f - t_s} e^{-\Delta m_Y(t_f - t_s)} \left[\frac{1}{2} + \frac{1}{4}(1 - e^{-\Delta m_Y}) \right] \\ & + \frac{A_{10}^{X \rightarrow Y}}{A_{00}^{X \rightarrow Y}} (-1)^{t_s} e^{-\Delta m_X t_s} \left[\frac{1}{2} + \frac{1}{4}(1 - e^{-\Delta m_X}) \right] \\ & + \frac{A_{11}^{X \rightarrow Y}}{A_{00}^{X \rightarrow Y}} (-1)^{t_f} e^{-\Delta m_X t_s - \Delta m_Y(t_f - t_s)} \left[\frac{1}{2} - \frac{1}{4}(e^{-\Delta m_Y} + e^{-\Delta m_X}) \right]. \end{aligned} \quad (3.4)$$

The terms in square brackets in Eq. (3.4) are the suppression factors for the oscillating state contributions. The $\Delta m_{X,Y}$ are the splittings between the ground-state masses and the opposite-parity masses, and their values can be computed precisely from fits to two-point correlators. We find values for these splittings in the range between about 0.1 and 0.4 in lattice units. With these values of the parameters the “same-sign” contributions [the third term in Eq. (3.4)] are suppressed by a factor of ~ 6 –20 by Eq. (3.2), where the suppression is greater at finer lattice spacings. The other oscillating-state contributions change sign as a function of t_s and are given by the first two terms in Eq. (3.4). These contributions are very small for our double ratio, and they are further suppressed by a factor of ~ 2 by the average in Eq. (3.2).

Figure 2 shows $R_{A_1}(t_s, t_f)$ and $R_{A_1}(t_s, t_f + 1)$ for two different, representative ensembles. One can see that the plateau is lower for odd total source-sink separation than for even total source-sink separation, whether the odd source-sink separation is larger or smaller than the even source-sink separation. This feature holds for all ensembles. It suggests that the “same-sign” oscillating states are visible in our data, and are comparable to, but somewhat larger than, our current statistical errors. The average of Eq. (3.2) suppresses this effect to around 0.1% on our coarser lattices and around 0.03% on our finest lattices. This effect is negligible compared to other errors. The fact that this effect is visible independently of whether the odd source-sink separation is larger or smaller than the even source-sink separation indicates

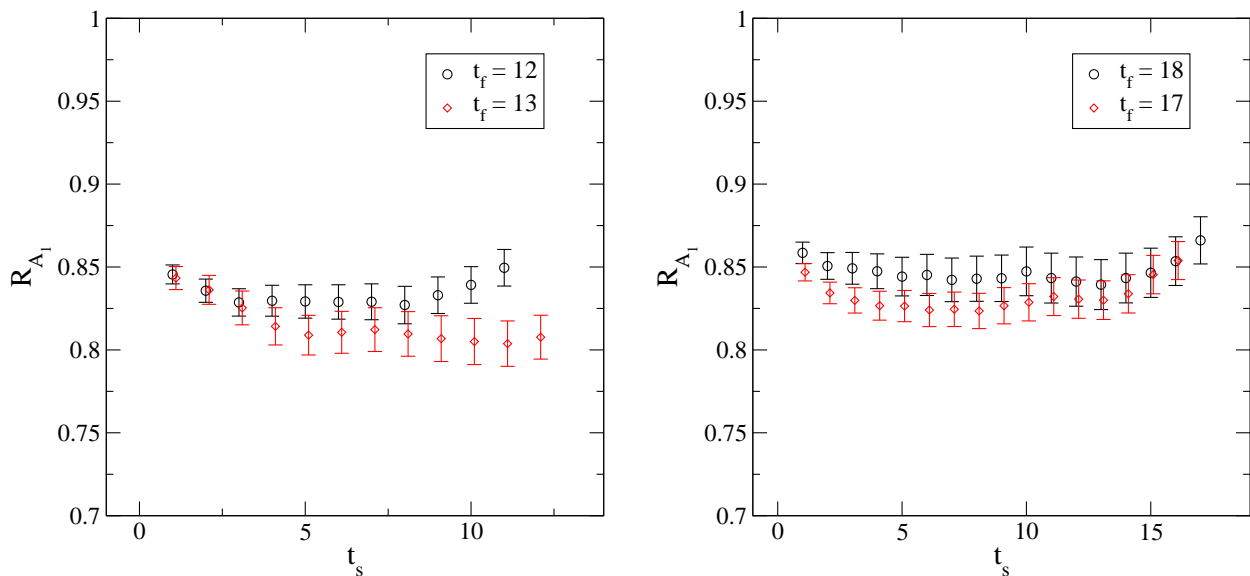


FIG. 2. R_{A_1} at $m_x = 0.2m'_s$ on coarse 0.12 fm (left) and on fine 0.09 fm (right) lattice spacings.

that this effect is larger than other excited-state contributions and that within the current statistical precision of our data, these can also be neglected.

The square-root of the average Eq. (3.2) is shown in Fig. 3 for coarse (0.12 fm), fine (0.09 fm), and superfine (0.06 fm) lattice spacings. These plots show data at unitary (full QCD) points, with valence spectator- and light sea-quark masses equal to $0.2m'_s$. The square-root of $\overline{R}_{A_1}(t_s, t_f)$ is fit to a constant in the identified plateau region, including the full covariance matrix to determine the correlated χ^2 and to ensure that the fits yielded acceptable p values. The fits are shown in Fig. 3 superimposed over the data with 1σ error bands. Source-sink separations and plateau ranges are approximately the same in physical units for all lattice spacings. Time ranges for fits, their p values, and the raw values for $h_{A_1}(1)$ are given in Table IV.

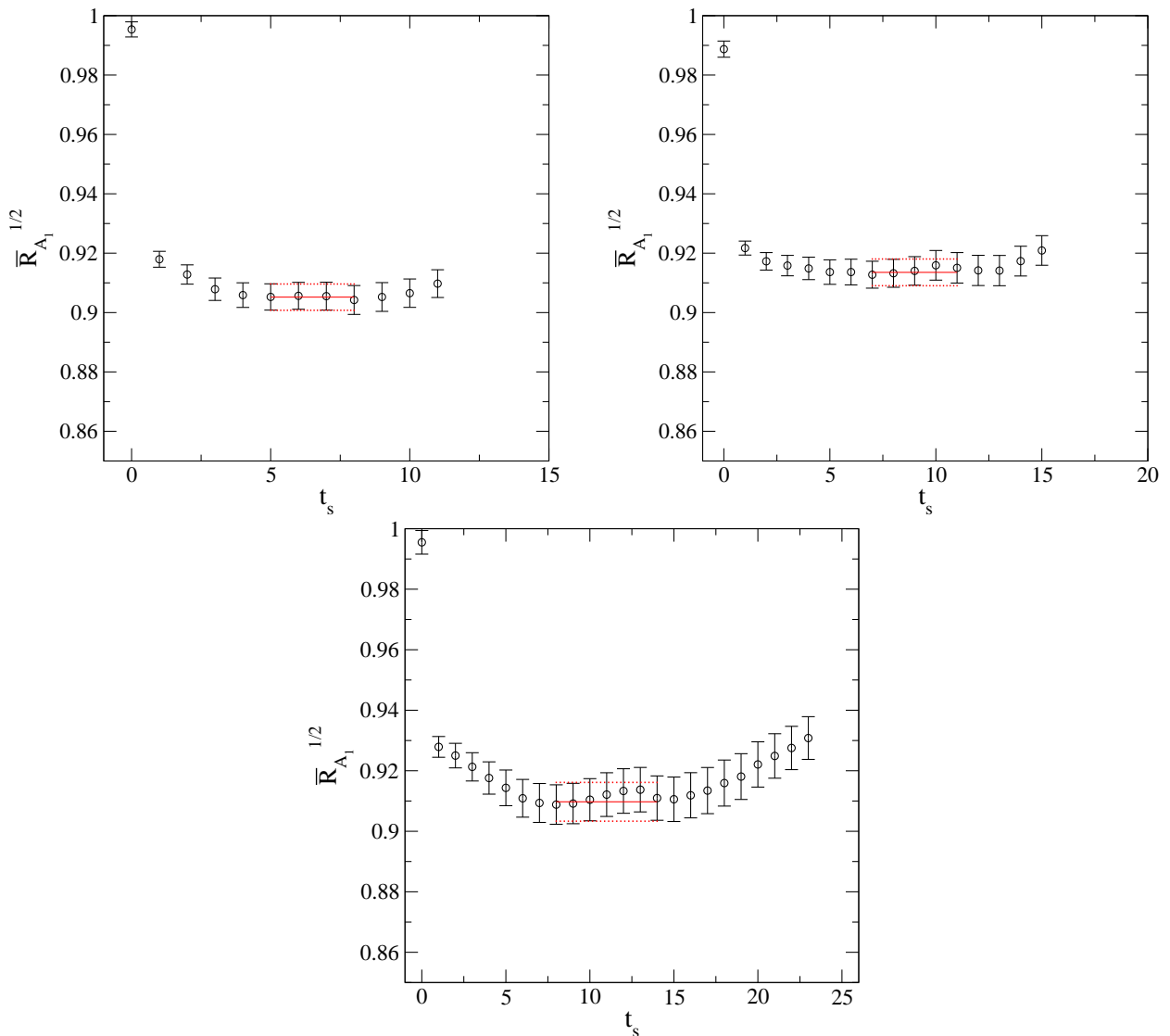


FIG. 3. $\overline{R}_{A_1}^{1/2}$ at $m_x = 0.2m'_s$ on coarse 0.12 fm (left), fine 0.09 fm (right), and superfine 0.06 fm (bottom). The plateau fits are shown with 1σ error bands.

TABLE IV. Fit results for double ratios at the full QCD points. The (approximate) lattice spacings a and the sea-quark masses $a\hat{m}'/am'_s$ (first two columns) identify the ensemble. The third column is the pair of spectator quark source-sink separations, the fourth is the time-slice fit range, the fifth is the p value of the fit, and the sixth is the value of $h_{A_1}(1)/\rho_{A^j}$ determined from the fit.

a (fm)	$a\hat{m}'/am'_s$	t_s	fit range	p value	$h_{A_1}(1)/\rho_{A^j}$
0.15	0.0097/0.0484	10, 11	5-7	0.85	0.9141(51)
0.12	0.02/0.05	12, 13	5-8	0.80	0.9035(28)
0.12	0.01/0.05	12, 13	5-8	0.97	0.9052(44)
0.12	0.007/0.05	12, 13	5-8	0.63	0.9160(53)
0.12	0.005/0.05	12, 13	5-8	0.68	0.9143(55)
0.09	0.0124/0.031	17, 18	7-11	0.63	0.9162(31)
0.09	0.0062/0.031	17, 18	7-11	0.54	0.9135(45)
0.09	0.00465/0.031	17, 18	7-11	0.78	0.9212(73)
0.09	0.0031/0.031	17, 18	7-11	0.95	0.9092(68)
0.09	0.00155/0.031	17, 18	7-11	0.79	0.9208(90)
0.06	0.0072/0.018	24, 25	8-14	0.84	0.9126(50)
0.06	0.0036/0.018	24, 25	8-14	0.93	0.9097(64)
0.06	0.0025/0.018	24, 25	8-14	0.13	0.9073(67)
0.06	0.0018/0.018	24, 25	8-14	0.55	0.9147(64)
0.045	0.0028/0.014	32, 33	7-14	0.87	0.9029(45)

IV. PERTURBATION THEORY FOR ρ_A

As discussed in Sec. II B, we need the ratio of matching factors, ρ_{A^j} , defined in Eq. (2.10). This ratio has been calculated in one-loop perturbation theory, which will be discussed in detail in another publication. The perturbative expansion for ρ_{A^j} is

$$\rho_{A^j} = 1 + \sum_{\ell} \rho_{A^j}^{[\ell]} \alpha_V^\ell(q^*), \quad (4.1)$$

where we make explicit a choice of scheme and scale for the perturbative series. The calculation of $\rho_{A^j}^{[1]}$ is a straightforward extension of the work in Ref. [54], modified to use the improved gluon propagator.

For the expansion parameter $\alpha_V(q^*)$, we would like to make a choice that prevents large logarithms associated with the β function from making the neglected terms unnecessarily large. Brodsky, Lepage, and Mackenzie [56] discussed how to do so by exploiting the n_f dependence of the second order in α_V , and Lepage and Mackenzie [57] explained how to define an equivalent scale choice when the second order is not yet available. The Lepage-Mackenzie version requires a coefficient $^*\rho_{A^j}^{[1]}$ defined by weighting the Feynman integral for $\rho_{A^j}^{[1]}$ with an additional factor of $\ln(q^2 a^2)$, where q is the gluon momentum in the one-loop diagram(s). Then the recommended (and empirically successful [57, 58]) scale q^* is given through

$$\ln(q^* a) = \frac{^*\rho_{A^j}^{[1]}}{2\rho_{A^j}^{[1]}}, \quad (4.2)$$

TABLE V. One-loop estimate of ρ_{Aj} . The first two columns label each ensemble with the approximate lattice spacing in fm and the sea simulation light- and strange-quark masses. The third column is $\alpha_V(q^*)$ with $q^* = 2/a$. The fourth column is ρ_{Aj} on that ensemble with statistical errors from the VEGAS evaluation of the one-loop coefficients.

a (fm)	$a\hat{m}'/am'_s$	$\alpha_V(q^*)$	ρ_{Aj}
0.15	0.0097/0.0484	0.3589	0.99422(4)
0.12	0.02/0.05	0.3047	0.99650(5)
0.12	0.01/0.05	0.3108	0.99623(5)
0.12	0.007/0.05	0.3102	0.99618(5)
0.12	0.005/0.05	0.3102	0.99617(5)
0.09	0.0124/0.031	0.2582	0.99978(4)
0.09	0.0062/0.031	0.2607	0.99963(4)
0.09	0.00465/0.031	0.2611	0.99957(4)
0.09	0.0031/0.031	0.2619	0.99950(4)
0.09	0.00155/0.031	0.2623	0.99946(4)
0.06	0.0072/0.018	0.2238	1.00334(3)
0.06	0.0036/0.018	0.2245	1.00323(3)
0.06	0.0025/0.018	0.2249	1.00317(3)
0.06	0.0018/0.018	0.2253	1.00312(3)
0.045	0.0028/0.014	0.2013	1.00608(2)

when the scheme is the V scheme, such that the interquark potential in momentum space is $C_F\alpha_V(q^2)/q^2$.

Unfortunately, as the heavy-quark masses vary over the range of interest, nearby zeroes of the numerator and denominator in Eq. (4.2) lead to physically unreasonable values for q^* . Fortunately, the way to deal with such cases has been spelled out by Hornbostel, Lepage, and Morningstar (HLM) [59]. The HLM method requires integrals weighted by higher powers of $\ln(q^2a^2)$. This prescription results in values for q_{HLM}^* that are close to $2/a$. We therefore use $q^* = 2/a$ to obtain the ρ_{Aj} listed in Table V. As expected, ρ_{Aj} varies somewhat as a function of lattice spacing. It is even slightly different from ensemble to ensemble at the same nominal lattice spacing, because these ensembles have slightly different lattice spacings.

V. HEAVY-QUARK MASS TUNING

Our approach to tuning $\kappa_{b,c}$ is similar to that described in Ref. [48], and a detailed description of the current approach is given in Appendix C. We start with the lattice dispersion relation

$$E^2(\mathbf{p}) = M_1^2 + \frac{M_1}{M_2}\mathbf{p}^2 + \frac{1}{4}A_4(a\mathbf{p}^2)^2 + \frac{1}{3}A_4a^2\sum_{j=1}^3|p_j|^4 + \dots, \quad (5.1)$$

where $M_1 \equiv E(\mathbf{0})$ defines the meson rest mass and the kinetic mass is given by

$$M_2^{-1} \equiv 2 \left. \frac{\partial E(\mathbf{p})}{\partial p_j^2} \right|_{\mathbf{p}=\mathbf{0}}. \quad (5.2)$$

TABLE VI. Errors in the tuned $\kappa_{b,c}$ parameters. The (approximate) lattice spacings a and the sea-quark masses $a\hat{m}'/am'_s$ (first two columns) identify the ensemble. The third and fourth columns are the tuned κ values for the b and c quarks, respectively. The first error is the statistics plus fitting error, and the second is an error due to the uncertainty in the lattice scale. The fifth and six columns are the κ values used in the simulations.

a (fm)	$a\hat{m}'/am'_s$	κ_b	κ_c	κ'_b	κ'_c
0.15	0.0097/0.0484	0.0775(16)(3)	0.12237(26)(20)	0.0781	0.1218
0.12	0.02/0.05	0.0879(9)(3)	0.12452(15)(16)	0.0918	0.1259
0.12	0.01/0.05	0.0868(9)(3)	0.12423(15)(16)	0.0901	0.1254
0.12	0.007/0.05	0.0868(9)(3)	0.12423(15)(16)	0.0901	0.1254
0.12	0.005/0.05	0.0868(9)(3)	0.12423(15)(16)	0.0901	0.1254
0.09	0.0124/0.031	0.0972(7)(3)	0.12737(9)(14)	0.0982	0.1277
0.09	0.0062/0.031	0.0967(7)(3)	0.12722(9)(14)	0.0979	0.1276
0.09	0.00465/0.031	0.0966(7)(3)	0.12718(9)(14)	0.0977	0.1275
0.09	0.0031/0.031	0.0965(7)(3)	0.12714(9)(14)	0.0976	0.1275
0.09	0.00155/0.031	0.0964(7)(3)	0.12710(9)(14)	0.0976	0.1275
0.06	0.0072/0.018	0.1054(5)(2)	0.12964(4)(11)	0.1048	0.1295
0.06	0.0036/0.018	0.1052(5)(2)	0.12960(4)(11)	0.1052	0.1296
0.06	0.0025/0.018	0.1051(5)(2)	0.12957(4)(11)	0.1052	0.1296
0.06	0.0018/0.018	0.1050(5)(2)	0.12955(4)(11)	0.1052	0.1296
0.045	0.0028/0.014	0.1116(3)(2)	0.130921(16)(7)	0.1143	0.1310

The meson masses differ from the corresponding quark masses, m_1 and m_2 , by binding-energy effects. In the Fermilab method, the lattice pole energy is fit to the dispersion relation Eq. (5.1), and κ is adjusted so that the kinetic mass agrees with experiment. We tune to the experimental D_s and B_s meson masses to obtain κ_c and κ_b , respectively.

The simulation values $\kappa'_{b,c}$ differ from our current best estimates of these parameters because of improvements in statistics and methodology since the initial tuning runs. Table VI shows our best estimates of $\kappa_{b,c}$, along with errors. The first error is a combination of statistical and fitting systematics, and the second error is that due to fixing the lattice scale. For comparison, Table VI also shows the $\kappa'_{b,c}$ values used in the runs. A detailed discussion of how the tuned values of $\kappa_{b,c}$ are obtained is given in Appendix C. As a cross-check of our tuning procedure, we calculate the hyperfine splittings $\Delta M(D_s) = M(D_s^*) - M(D_s)$ and $\Delta M(B_s) = M(B_s^*) - M(B_s)$. In Appendix C 4 we find

$$\Delta M(D_s) = 146 \pm 4 \text{ MeV}, \quad \Delta M(B_s) = 44 \pm 3 \text{ MeV}, \quad (5.3)$$

where the error includes statistics and the sum of all systematic errors in quadrature. These are in good agreement with the experimental values $\Delta M(D_s) = 143.8 \pm 0.4 \text{ MeV}$ and $\Delta M(B_s) = 48.7_{-2.1}^{+2.3} \text{ MeV}$.

We correct our values of $h_{A_1}(1)$ for the mistuning of κ using information on the heavy-quark mass dependence from an additional run with $\kappa'_{b,c}$ nearer their physical values on the coarse ensemble with $a\hat{m}'/am'_s = 0.01/0.05$. To apply the correction we exploit information from heavy-quark effective theory (HQET); the form factor at zero-recoil has the heavy-

quark expansion [60, 61]

$$h_{A_1}(1) = \eta_A \left[1 - \frac{\ell_V}{(2m_c)^2} + \frac{2\ell_A}{2m_c 2m_b} - \frac{\ell_P}{(2m_b)^2} \right], \quad (5.4)$$

up to order $1/m_Q^2$, where η_A is a factor that matches HQET to QCD and the ℓ 's are long-distance matrix elements of the HQET. Heavy-quark symmetry forbids terms of order $1/m_Q$ at zero-recoil [62]. The form factor depends on both the bottom quark mass and the charm quark mass; we correct for this dependence and propagate the uncertainty due to the error in $\kappa_{b,c}$ to the form factor before performing the chiral/continuum extrapolation. The leading m_b dependence is given by the term that is inversely proportional to $m_c m_b$ in brackets in Eq. (5.4), and this dependence, inversely proportional to m_b for fixed charm-quark mass, is the one used to correct the form factor for the mistuning in m_b . The leading charm-quark mass dependence is, however, given by the term that is inversely proportional to the charm quark mass squared. Thus, we determine the adjustment that must be made from the simulated form factor h_{sim} to the tuned value h_{tuned} using

$$h_{\text{tuned}} = h_{\text{sim}} + \frac{\partial h}{\partial[1/(r_1 m_b)]} \left[\frac{1}{r_1 m_{b,\text{tuned}}} - \frac{1}{r_1 m_{b,\text{sim}}} \right] + \frac{\partial h}{\partial[1/(r_1 m_c)^2]} \left[\frac{1}{(r_1 m_{c,\text{tuned}})^2} - \frac{1}{(r_1 m_{c,\text{sim}})^2} \right], \quad (5.5)$$

where $m_{b,c}$ is the kinetic b or c quark mass, and r_1 sets the relative lattice spacing on different ensembles. The slope parameters are determined by a linear interpolation between the two sets of points shown in Fig. 4. One of these points in each of these plots is from our original production run, while the other points are from runs where $\kappa_{b,c}$ were separately varied and chosen to be closer to their tuned values.

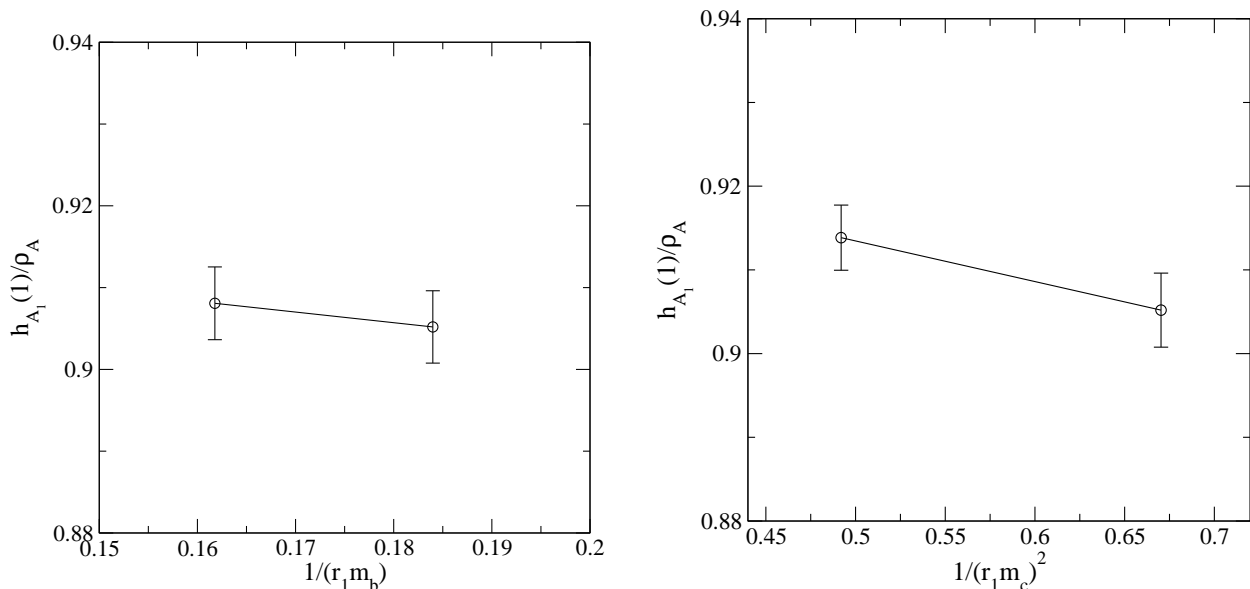


FIG. 4. $h_{A_1}(1)$ at different values close to the tuned b and c quark masses. Each is plotted as a function of the leading (assuming m_b is sufficiently heavier than m_c) heavy-quark mass dependence in Eq. (5.4), $1/(r_1 m_b)$ and $1/(r_1 m_c)^2$ for b and c , respectively.

The slopes are also used to propagate the errors in the tuned kappa values due to “statistics and fitting” to the errors in each individual $h_{A_1}(1)$ data point before performing the chiral/continuum extrapolation. This is done by inflating the jackknife error of $h_{A_1}(1)$ on each data point by adding to it in quadrature the parametric error in $h_{A_1}(1)$ due to the “statistics and fitting” part of the κ tuning error. We make the assumption that the statistics and fitting errors in the tuned κ values on different ensembles are independent of one another, though we also test the size of the additional error induced if this assumption is not true and find that it is small. The κ tuning “statistics and fitting” error is thus directly incorporated into the statistical error of h_{A_1} . The scale error in the tuned κ values, however, is 100% correlated across ensembles, and is therefore treated as a separate systematic error.

VI. CHIRAL-CONTINUUM EXTRAPOLATION

Because the light u and d -quark masses used in the calculation are heavier than the physical ones, an extrapolation in quark mass is necessary. This extrapolation can be controlled using an appropriate chiral effective theory, where one can also incorporate discretization effects particular to staggered quarks. The chiral effective theory that incorporates these effects is rooted staggered chiral perturbation theory (rS χ PT), which was extended to include heavy-light quantities in Ref. [63].

There are discretization effects that are particular to staggered quark actions. The staggered quark discretization only partially solves the fermion doubling problem, reducing the number of species from 16 to 4. There remain unphysical species of quarks, commonly referred to as tastes. Quarks of different tastes can exchange high momentum gluons with momenta of order the lattice cutoff, and this exchange breaks the degeneracy in the pion spectrum for pions made of quarks of different tastes. This taste-symmetry breaking leads to the staggered theory having 16 light pseudoscalar mesons instead of 1.

The tree-level relation in the chiral theory between the pseudoscalar meson masses and the quark masses is given by

$$M_{xy,\xi}^2 = B_0(m_x + m_y) + a^2\Delta_\xi, \quad (6.1)$$

where ξ labels the meson taste, m_x and m_y are the staggered quark masses, B_0 is the continuum low-energy constant, and $a^2\Delta_\xi$ are the splittings of the 16 tastes. An additional SO(4) taste-symmetry, which is broken only at $O(a^4)$, leads to some degeneracy among the 16 pions, such that the taste index ξ runs over the multiplets P, A, T, V, I with degeneracies 1, 4, 6, 4, 1, respectively. The splitting $a^2\Delta_P$ vanishes because of an exact nonsinglet lattice axial symmetry.

Eq. (34) of Ref. [64] gives the result for $h_{A_1}(1)$ in partially-quenched χ PT with degenerate up and down quark masses (the 2+1 case) in the rooted staggered theory. The result is

$$\frac{h_{A_1}^{(B_x)PQ,2+1}(1)}{\eta_A} = 1 + \frac{X_A(\Lambda_\chi)}{m_c^2} + \frac{g_{D^*D\pi}^2}{48\pi^2 f^2} \times \text{logs}_{1\text{-loop}}(\Lambda_\chi), \quad (6.2)$$

where the term $\text{logs}_{1\text{-loop}}(\Lambda_\chi)$ stands for the one-loop staggered chiral logarithms, the detailed expression for which is given in Appendix A. $X_A(\Lambda_\chi)$ is a low-energy constant of the chiral effective theory, independent of the light-quark mass, and its dependence on the chiral scale Λ_χ cancels that of the chiral logarithms. The $X_A(\Lambda_\chi)$ term is suppressed by a factor of $1/m_c^2$ in the heavy-quark power counting. The term η_A is a factor that matches HQET to QCD,

TABLE VII. Parameters used in the chiral extrapolation, including the staggered taste-splittings for the different taste mesons. The first column is the approximate lattice spacing, and the second through fifth columns are the taste-splittings for the taste scalar, axial-vector, tensor, and vector mesons, respectively. The sixth column is the tree-level low energy constant appearing in Eq. (6.1).

a (fm)	$r_1^2 a^2 \Delta_I$	$r_1^2 a^2 \Delta_A$	$r_1^2 a^2 \Delta_T$	$r_1^2 a^2 \Delta_V$	$r_1 B_0$
0.15	0.9851	0.7962	0.6178	0.3915	6.761
0.12	0.6008	0.4803	0.3662	0.2270	6.832
0.09	0.2207	0.1593	0.1238	0.0747	6.639
0.06	0.0704	0.0574	0.0430	0.0263	6.487
0.045	0.0278	0.0227	0.0170	0.0104	6.417

TABLE VIII. Values of physical quark masses and $r_1 B_0$ with discretization errors removed in a mass independent scheme. The masses are in units of the 0.09 fm lattice spacing with the 0.09 fm lattice value of the mass renormalization. The first column is the physical s quark mass, the second is the average of the u and d quark masses, the third is the u quark mass, and the fourth is the d quark mass. The fifth column is the value of the low energy constant $r_1 B_0$ evaluated at the same scale within the same scheme and with discretization errors removed.

$am_s \times 10^2$	$a\hat{m} \times 10^3$	$am_u \times 10^3$	$am_d \times 10^3$	$r_1 B_0$
2.65(8)	0.965(33)	0.610(26)	1.32(5)	6.736

and contains perturbative-QCD logarithmic dependence on the heavy-quark masses. It is independent of the light-quark mass. The coefficient of the chiral logarithm term contains f , the pion decay constant and $g_{D^*D\pi}$, the $D^*D\pi$ coupling in the chiral effective theory.

The one-loop logarithm term depends on the light valence- and sea-quark masses, including the taste-breaking discretization effects from the light-quark sector. The expression contains explicit dependence on the lattice spacing a , and requires as inputs the parameters of the staggered chiral Lagrangian δ'_V and δ'_A , which are determined from chiral fits to pion masses and decay constants on the same ensembles. The chiral formula for $h_{A_1}(1)$ also requires as input the taste-splittings Δ_ξ , which are obtained from separate spectrum calculations of the various taste mesons. The values of the staggered taste-splittings are given in Table VII. We take the values of the hairpin parameters δ'_V and δ'_A on the $a \approx 0.12$ fm lattices to be $r_1^2 a^2 \delta'_V = 0.00$ and $r_1^2 a^2 \delta'_A = -0.28$. Their values at other lattice spacings are determined by scaling these numbers by the ratio of the root-mean-square splitting at the target lattice spacing and at $a \approx 0.12$ fm. We find that varying the staggered parameters within their uncertainties produces a negligible error in h_{A_1} , as further discussed in Section VII C. The continuum low-energy constant $g_{D^*D\pi}$ is taken as an input in our fits. We take a value with an error that encompasses recent lattice-QCD calculations and the latest measurements of the D^* decay width (See Sec. VII C for details). The D^*-D mass splitting $\Delta^{(c)}$ is well determined from experiment. In summary, the only free parameter in the next-to-leading order (NLO) chiral formula is the constant $X_A(\Lambda)$, which is determined by fits to our lattice data for the form factor $h_{A_1}(1)$.

The errors in the light quark masses lead to negligible uncertainty in h_{A_1} ; these masses are presented in Table VIII in the ‘‘continuum,’’ where the values have been extrapolated to the continuum, i.e. discretization errors have been removed. The masses are in units of

the 0.09 fm lattice spacing with the 0.09 fm lattice value of the mass renormalization in a mass independent scheme. The value of $r_1 B_0$ evaluated at the same scale within the same scheme and with discretization errors removed is also given in Table VIII.

Table IX shows our results for the lattice form factor $h_{A_1}(1)$ for various light-quark masses on the different ensembles. We computed the form factor at the full QCD points on all of the ensembles, and on some of the ensembles we included a partially quenched point with the spectator light-quark mass equal to $0.4m'_s$ in order to help constrain the fits. Because these points have small statistical errors due to the heavier spectator-quark mass, they are especially useful in constraining the lattice-spacing dependence. Table IX also presents the values of the pion mass corresponding to the light spectator-quark mass for the full QCD points. Both the pseudoscalar-taste pion mass and the root-mean-square pion mass are given. Note that the RMS and Goldstone pion masses presented in Table IX use the mass-independent determination of r_1/a to fix the relative lattice scale, and thus differ somewhat from an earlier set of masses on the same ensembles appearing in supporting material of the Flavor Lattice Averaging Group [65]. This earlier set of masses used mass-dependent r_1/a values to set the relative scale. As Table IX shows, our lightest taste-Goldstone pion mass is 180 MeV, while the lightest root-mean-squared (RMS) pion mass is 260 MeV. Previous work on MILC ensembles [22, 66] suggests that when masses in these ranges are combined with staggered χ PT then the systematic error from the resulting chiral/continuum extrapolation can be estimated reliably. Although staggered χ PT allows us to remove the leading discretization effects from the light quarks, the heavy-quark discretization effects are more complicated; see Appendix B for details.

If we restrict ourselves to a strictly NLO χ PT (one-parameter) fit we find a not-so-good p value of 0.05, but if we modify our fit so that it includes the NLO terms and a free parameter proportional to a^2 [a next-to-next-to-leading order (NNLO) analytic term] then we find a reasonably good p value of 0.25. We find even better fits if we include all analytic terms through NNLO. We do not include the NNLO logarithms because they are unknown and would require a two-loop calculation. The fit expression including all analytic NNLO terms is

$$\frac{h_{A_1}^{\text{NNLO}}(1)}{\eta_A} = c_0 + \text{NLO}_{\log s} + c_1 m_{X_P}^2 + c_2(2m_{U_P}^2 + m_{S_P}^2) + c_3 a^2, \quad (6.3)$$

where the subscript P on the meson masses indicates the taste pseudoscalar mass. The fit parameter c_0 represents the quantity $1 + X_A(\Lambda_\chi)/m_c^2$ appearing on the right-hand side of Eq. (6.2), while $\text{NLO}_{\log s}$ is a short-hand expression for the last term on the right-hand side of Eq. (6.2). By heavy-quark symmetry, the c_i are suppressed by a factor of $1/m_c^2$. The one-loop corrections start at $\mathcal{O}(\bar{\Lambda}^2/m_Q^2)$ so that one has to go to NNLO to find terms of $\mathcal{O}[(\bar{\Lambda}^2/m_Q^2)p^2]$. In order to estimate systematic errors we try adding a variety of even higher-order analytic terms to this expression, as described in detail in Section VII C. We prefer to take a central value for the extrapolated form factor that is roughly in the middle of the range of results from the various alternative fits used to estimate our central value. The motivation for this form is no greater than for the other fits that were tried. Our preferred central value fit is to the form

$$\frac{h_{A_1}^{\text{NNLO}}(1)}{\eta_A} = c_0 + \text{NLO}_{\log s} + c_1 m_{X_P}^2 + c_2(2m_{U_P}^2 + m_{S_P}^2) + c_3 a^2 + c_4 m_{X_P}^4, \quad (6.4)$$

which, in addition to the analytic NNLO terms of Eq. (6.3), includes an NNNLO term proportional to $m_{X_P}^4$. Because the various fit Ansätze for $h_{A_1}(1)$ considered have at most six free

TABLE IX. Results for $h_{A_1}(1)$ at various light-quark masses, including partially-quenched points. The (approximate) lattice spacings a and the sea-quark masses $a\hat{m}'/am'_s$ identify the ensemble (first two columns). The third column labels the valence spectator-quark mass. The fourth and fifth columns are the approximate taste-Goldstone and root-mean-square pion masses associated with the valence spectator mass (values are only given for the unitary points). The sixth column is the value of $h_{A_1}(1)$ at that valence mass (corrected for κ mistuning and including the perturbative matching factor). The error on $h_{A_1}(1)$ is statistical only.

a (fm)	$a\hat{m}'/am'_s$	am_x	$M_{\pi,P}$ (MeV)	$M_{\pi,RMS}$ (MeV)	$h_{A_1}(1)$
0.15	0.0097/0.0484	0.0097	340	590	0.9077(52)
0.15	0.0097/0.0484	0.0194	-	-	0.9085(35)
0.12	0.02/0.05	0.02	560	670	0.9068(29)
0.12	0.01/0.05	0.01	390	540	0.9068(45)
0.12	0.01/0.05	0.02	-	-	0.9068(30)
0.12	0.007/0.05	0.007	320	500	0.9175(53)
0.12	0.007/0.05	0.02	-	-	0.9131(28)
0.12	0.005/0.05	0.005	270	470	0.9158(56)
0.12	0.005/0.05	0.02	-	-	0.9108(28)
0.09	0.0124/0.031	0.0124	500	550	0.9180(32)
0.09	0.0062/0.031	0.0062	350	420	0.9155(46)
0.09	0.0062/0.031	0.0124	-	-	0.9147(31)
0.09	0.00465/0.031	0.00465	310	380	0.9227(73)
0.09	0.0031/0.031	0.0031	250	330	0.9108(69)
0.09	0.0031/0.031	0.0124	-	-	0.9125(37)
0.09	0.00155/0.031	0.00155	180	280	0.9227(90)
0.06	0.0072/0.018	0.0072	450	470	0.9142(51)
0.06	0.0036/0.018	0.0036	320	340	0.9127(65)
0.06	0.0036/0.018	0.0072	-	-	0.9130(45)
0.06	0.0025/0.018	0.0025	260	290	0.9105(88)
0.06	0.0018/0.018	0.0018	220	260	0.9182(65)
0.045	0.0028/0.014	0.0028	320	330	0.9121(46)

parameters, we do not need to impose constraints on any of the unknown coefficients. The coefficients are of the size expected from power counting in heavy-meson chiral perturbation theory.

Our preferred central value fit is shown in Fig. 5, where the curves show the light-quark mass dependence at different lattice spacings. The cyan band is the continuum extrapolated result. A notable feature of the chiral extrapolation is a cusp that appears close to the physical pion mass. The cusp is due to the presence of the $D\pi$ threshold and the fact that the D - D^* splitting is very close to, but slightly larger than, the physical pion mass. One can see from the curves in Fig. 5 that the cusp is expected to be washed out by finite-lattice-spacing effects, but is recovered in the continuum limit. The p value for this fit is 0.78; the alternative fits that also include higher-order analytic terms have similar p values. Figure 6 shows nearly the same plot, but with only the continuum curve displayed. The extrapolated

value for the form factor is also shown, including the full systematic error for our final result.

VII. SYSTEMATIC ERRORS

In this section, we examine the uncertainties in our calculation in detail. Statistical uncertainties are computed with a single elimination jackknife and fits use the full covariance matrix to determine χ^2 . We devote a subsection to each of the sources of uncertainty: fitting and excited states, the heavy-quark mass and lattice-scale dependence, the chiral extrapolation of the light spectator-quark mass (in particular the $D^*-D-\pi$ coupling), discretization errors, perturbation theory, and isospin effects.

A. Fitting and excited states

We determine plateau fits to the double ratio, Eq. (2.12). The fits are done under a single elimination jackknife, after blocking the data by 4 on all ensembles. The χ^2 is defined using the full covariance matrix. Statistical errors are determined in fits that include the full correlation matrix, which was remade for each jackknife fit. In order to correctly propagate the correlated statistical errors to the chiral/continuum extrapolation fits, the jackknife data sets on different ensembles are combined into a larger block-diagonal jackknife data set. The

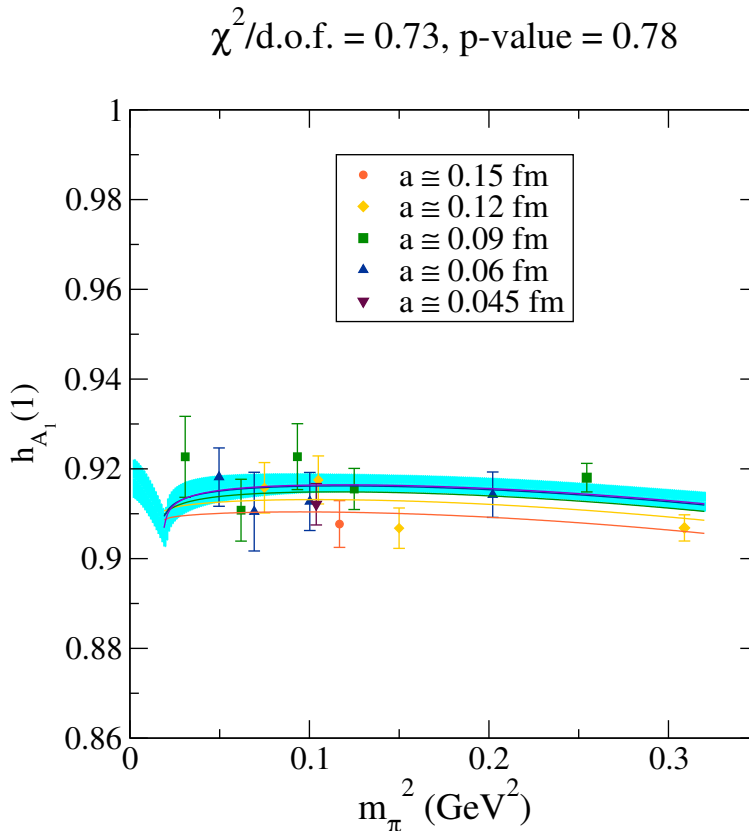


FIG. 5. The full QCD points for $h_{A_1}(1)$ versus m_π^2 at five lattice spacings are shown in comparison to the continuum curve and the various fit curves.

block size of 4 is chosen only to keep the combined data set to a manageable size for the chiral and continuum extrapolation fits. We find that the statistical errors do not grow with blocking, and that therefore the autocorrelation errors are negligible even without blocking. This was not true in our previous calculation [7], although that calculation used many of the same ensembles. This is because in the current calculation, we move the source origin around the lattice randomly, whereas in the previous calculation the source origin was fixed.

With several hundred configurations on each ensemble, and over two thousand configurations on some ensembles, we do not have difficulty resolving the full covariance matrix in our correlator fits, and we do not need to resort to a singular value decomposition cut on the eigenvalues of the covariance matrix. We find that the averaged ratio data (constructed from our correlators using Eq. (3.2)) on the 0.09 fm lattices are well-described by a fit to a constant over a range of 5 time slices, and that the fit range where an acceptable fit is obtained is roughly the same in physical units across ensembles. The correlated $\chi^2/\text{d.o.f.}$ ranges from 0.08 to 0.85, with one exception. On the 0.06 fm, $0.15m_s$ ensemble, the $\chi^2/\text{d.o.f.}$ is 1.71, a bit higher than one might expect, based on fits to the same physical time range on other ensembles. Also, the double ratio $R(t)$ appears somewhat asymmetric under the interchange of source and sink on this ensemble, but this must be a statistical fluctuation, since $R(t)$ is symmetric by construction. For this ensemble, we adopt the Particle Data Group (PDG) prescription and rescale the statistical error by the square root of the $\chi^2/\text{d.o.f.}$ Time ranges for fits, their p values, and the raw values for $h_{A_1}(1)$ are given in Table IV. We take the good quality of our results compared to other

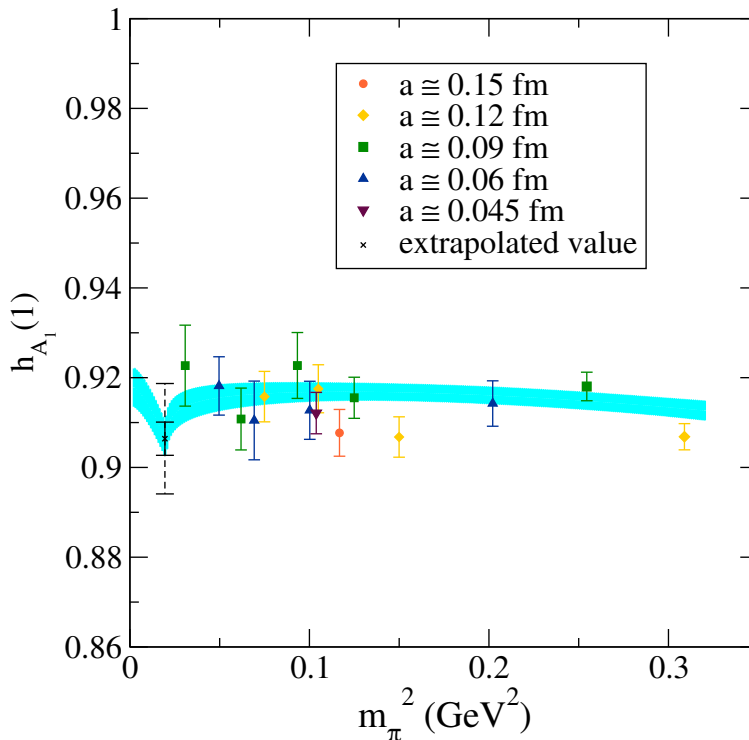


FIG. 6. The full QCD points for $h_{A_1}(1)$ versus m_{π}^2 at five lattice spacings are shown in comparison to the continuum curve. The cross is the extrapolated value, where the solid line is the statistical error, and the dashed line is the total systematic error added to the statistical error in quadrature.

we assign no further error to fitting and excited states.

B. Heavy-quark mass and lattice-scale dependence

As discussed in Sec. V, the simulation values for $\kappa_{b,c}$ differ from the best tuned values for these quantities, since the initial tuning analysis was supplemented by additional data and improved methodology. We use Eq. (5.5) to perform the shift in the form factor given the tuned values of $\kappa_{b,c}$ in Table VI. The dependence of h_{A_1} on κ (or m_2) can also be used to propagate the errors in κ shown in Table VI to the form factor. This is done by inflating the difference from the mean under a jackknife for the data points on different ensembles. The inflation factor is the sum in quadrature of the statistical error and the parametric error in h_{A_1} due to the κ uncertainty labeled “statistics and fitting” only. Thus, the statistical error in h_{A_1} includes the “statistics and fitting” error in the κ tuning. The error in the determination of $\kappa_{b,c}$ coming from setting the lattice scale is treated separately below.

This treatment of the heavy-quark mass tuning error assumes that the errors in κ are independent for each ensemble. The error would be larger if the adjustment in the form factor varied systematically across multiple ensembles. To test the size of such a systematic error, we redo the central fit with all of the coarse ensembles shifted together by 1σ of the estimated errors in $\kappa_{b,c}$. This leads to a small shift in the central value which is negligible compared to other errors. The errors in $dh/d[1/(r_1 m_b)]$ and in $dh/[(r_1 m_c)^2]$ are negligible compared to the other heavy-quark mass tuning errors.

The relative lattice spacing between different ensembles is fixed in units of r_1/a . The absolute lattice spacing is then fixed using the MILC determination of $r_1 = 0.3117(22)$ fm from f_π [51]. Because the form factor is dimensionless, the error in setting the lattice scale mainly affects $h_{A_1}(1)$ by introducing an uncertainty in the determination of the bare b - and c -quark masses. Changing r_1 within its error of approximately 0.7% leads to an additional 0.1% systematic error in $h_{A_1}(1)$.

C. Chiral extrapolation

We estimate the systematic error due to the chiral extrapolation by comparing various types of fits including analytic terms of higher order than NLO in rS χ PT, since the two-loop NNLO logarithms are unknown. We also compare with continuum χ PT, where staggered effects are removed from the one-loop logarithms. Finally, we account for additional errors that appear due to the uncertainties in the parameters that enter the NLO rS χ PT expression. The largest of these is the uncertainty in $g_{D^*D\pi}$, the coupling between the D^* , D , and π in the (continuum) chiral effective theory. As emphasized in our previous calculation of the $B \rightarrow D^* \ell \nu$ form factor [7], the chiral logarithms are of order 10^{-3} in the region where we have data, and the nonanalytic behavior is only important near the physical pion mass. In that region, χ PT is expected to provide a good description of the physics. This is important, because very near the physical pion mass there is a cusp in the form factor. This is due to the presence of the $D\pi$ threshold and the fact that the D - D^* splitting is so close to the physical pion mass. Because this cusp is a physical effect, it should be included in any version of the chiral extrapolation that is used to estimate systematic errors.

Through NLO order (one-loop) in rS χ PT there is only one free parameter, an overall constant. The other parameters that appear in the continuum expression through one-loop

are determined from either the lattice or phenomenology. They are $g_{D^*D\pi}$, f_π , m_π , and the D - D^* mass splitting $\Delta^{(c)}$. The constants f_π and $g_{D^*D\pi}$ appear in an overall multiplicative factor $g_{D^*D\pi}^2/48\pi^2 f_\pi^2$ in front of the logarithmic term; see Eq. (A1). The main uncertainty in the size of the cusp comes from the uncertainties of these one-loop input parameters. The parameters f_π , $\Delta^{(c)}$, and the pion mass itself are all precisely determined from experiment, and contribute only small errors to the overall determination of the size of the cusp. The dominant error in the size of the cusp comes from the uncertainty in $g_{D^*D\pi}$.

There are additional parameters that enter the one-loop rS χ PT expression due to lattice artifacts. These are the taste splittings $a^2\Delta_\xi$ with $\xi = P, A, T, V, I$, and the taste-violating hairpin-coefficients $a^2\delta'_A$ and $a^2\delta'_V$. The former are well-determined from staggered meson spectrum calculations, and the latter are determined from simultaneous rS χ PT fits to $m_\pi^2/(m_x + m_y)$ and f_π . Because the chiral logarithms are such a small contribution to the fit form in the region where we have data, it makes essentially no difference whether we include the modifications for staggered fermions or not. We see no difference in the extrapolated continuum result when comparing staggered and continuum χ PT fit results through 4 decimal places. Thus, the uncertainties in the parameters specific to rS χ PT are negligible in our extrapolation.

We find that a fit to the NLO expression supplemented by a term linear in a^2 , does an adequate job of fitting the data, with $\chi^2/\text{d.o.f.} = 1.20$ corresponding to $p = 0.25$. The quality of the fit can be improved either by pruning the heaviest mass points or by adding higher-order analytic terms to the fit function; we try both. For our central value we choose a fit that falls around the middle of the range of all the fits that we have tried. For our error, we take the largest difference between the central value and the different alternatives. Our preferred central value fit is to Eq. (6.4), which, in addition to the analytic NNLO terms of Eq. (6.3), includes an NNNLO term proportional to $m_{X_P}^4$. Alternative fits with good p values include the following: Eq. (6.4) without the c_4 term, Eq. (6.4) with an additional term $c_6 a^2(2m_{U_P}^2 + m_{S_P}^2)$, repeating these fits but taking only the ensembles with $a \leq 0.09$ fm. This cut on the lattice spacing also cuts out the data with the heaviest pion masses, as can be seen in Table IX. We also considered a fit that tests for the presence of higher-order taste-breaking effects. This fit is similar to the central value fit but with the taste-pseudoscalar pion mass in the analytic terms replaced by the taste-tensor pion mass (which is close to the root-mean-square pion mass). The largest variation from the central value of the form factor in all of these fits is 0.0049, or 0.5%. Figure 6 shows all of the full QCD points in our calculation as a function of (taste-Goldstone) pion mass, as well as the continuum extrapolated curve and the extrapolated value for $h_{A_1}(1)$ with the full systematic error.

The largest of the parametric uncertainties in our chiral extrapolation is that due to the chiral-Lagrangian coupling $g_{D^*D\pi}$, which sets the size of the cusp. Our data do not constrain it, so we must take its value from elsewhere. New lattice calculations of $g_{D^*D\pi}$ [67, 68] have appeared since our previous work on $B \rightarrow D^*\ell\nu$. In Ref. [67], 2 light flavors of quarks were included in the sea, but otherwise the systematic errors appear to be under control. The authors find $g_{D^*D\pi}(N_f = 2) = 0.53(3)(3)$, where the first error is statistical and the second is systematic error due to chiral extrapolation. The calculation in Ref. [68] includes 2+1 light dynamical flavors, but only a single lattice spacing. The authors find $g_{D^*D\pi} = 0.55(6)$, consistent with the 2-flavor calculation. These results are also consistent with the values extracted from the experimental measurements of the D^* decay width [69–71]. A new preliminary 2+1 flavor result for the analogous coupling in the B system reports $g_{B^*B\pi} = 0.569(48)(59)$ [72]. Finally, a 2+1 flavor calculation of the coupling in the static

heavy-quark limit [73] finds, after a careful study of systematic effects, $g_{\text{static}} = 0.449(51)$. Although the result of Ref. [67] is a calculation directly at the charm quark mass, it only has two flavors of sea quarks, so we take an error that encompasses that of the 2+1 flavor result in the static limit in order to be conservative. Thus, in our fits we take $g_{D^*D\pi} = 0.53 \pm 0.08$, leading to a parametric, systematic uncertainty in $h_{A_1}(1)$ of 0.3%.

The size of the cusp is also expected to be modified by terms of higher order in the chiral expansion, *i.e.*, the two-loop chiral logarithms. Although possible higher-order corrections are at least partially accounted for by our analytic terms in the range of pion masses where we have data, the cusp is entirely determined by the chiral effective theory, so it is important to consider how that prediction might be affected by higher-order corrections independent of the analytic terms that we have added. Because the effect occurs very near the physical pion mass, we expect the relevant power counting to be that of $SU(2)_L \times SU(2)_R$ χ PT. We estimate the potential size of the two-loop corrections to the cusp by considering the size of the one-loop corrections to f_π compared to its $SU(2)$ chiral limit value f_2 , since these one-loop corrections to a parameter appearing in the coefficient of the one-loop term are expected to be typical of the size of the other two-loop corrections. We take the most recent value for $f_\pi/f_2 = 1.062(3)$ from the MILC Collaboration [74] and find that a 6% change in f_π leads to a 0.1% change in $h_{A_1}(1)$. Thus, for our chiral extrapolation error we include an additional 0.1% systematic error due to higher-order chiral corrections to the cusp added in quadrature with the 0.5% systematic error estimated from the spread in reasonable fits discussed above.

All other parametric uncertainties in the chiral formulas can be neglected. The physical pion mass in the chiral extrapolation is taken from experiment, so the errors from the uncertainties in the low-energy constant B_0 in Eq. (6.1) and in the light-quark masses are negligible. We take the charm meson mass splitting $\Delta^{(c)}$ from experiment, and the error due to its uncertainty is also negligible. Changing the (bare) strange quark mass within its error of approximately 2% also has a negligible effect on $h_{A_1}(1)$.

D. Finite-volume effects

The finite-volume effects can be estimated using heavy-light χ PT, where the integrals are replaced by discrete sums. The corrections to the integrals in the formulas appearing for $B \rightarrow D^*$ decays were worked out by Arndt and Lin [75]. Although the finite-volume effects would be large very near the cusp at the physical pion mass on the ensembles we are using (ranging in size from 2.5–5.5 fm), for the values we have actually simulated, the finite-size effects predicted by χ PT are less than one part in 10^4 . This is not a result of any particular cancellation, but rather due to the very small contribution of the chiral logarithms to this quantity. Thus, the finite-size effects are expected to be negligible for our calculation, and we do not assign any additional error due to them.

E. Discretization errors

Figure 7 shows the dependence of $h_{A_1}(1)$ as a function of a^2 , for fixed spectator-quark mass. The observed lattice-spacing dependence is, at most, as large as the statistical error. The HQET theory of heavy-quark discretization effects anticipates this small size but does not, however, predict a simple power-series for the a dependence, making a naive ex-

trapolation problematic. In Appendix B, we present a detailed analysis for the expected a dependence. In short, we expect the overall size of heavy-quark discretization errors to be of order $a\bar{\Lambda}^2/m_c$ and $a^2\bar{\Lambda}^2$, but must choose a value of $\bar{\Lambda}$. We compare the observed variation with a^2 of the data in Fig. 7 with the theory [53, 54]. We find that if we choose $\bar{\Lambda} = 450$ MeV, then the theoretical estimates are compatible with the data’s a dependence. In this way, we deduce that the discretization error on the superfine lattice ($a \approx 0.060$ fm) is 1%, leading to the row labeled “discretization errors” in Table X.

F. Perturbation theory

The calculation of ρ_{Aj} defined in Eq. (2.10) is carried out at one-loop order in perturbation theory, as discussed in Sec. IV. Because ρ_{Aj} is defined from a ratio of current renormalization factors, its deviation from unity is expected to be small by construction. Indeed, the one-loop corrections to ρ_{Aj} shown in Table V confirm our expectation. They range from 0.05% to 0.6%. In order to estimate the error due to the omitted higher-order corrections, we consider the variation of the one-loop corrections to ρ_{Aj} with the quark masses used in this calculation. We also consider the related renormalization factor ρ_{V^4} , defined from the charm-bottom vector current V_{cb}^4 analogously to the definition of ρ_{Aj} in Eq. (2.10). We find $\rho^{[1]} \leq 0.1$ for both currents. We then estimate the uncertainty as $\rho_{\max}^{[1]} \cdot \alpha_s^2$ with $\rho_{\max}^{[1]} = 0.1$ and $\alpha_s = \alpha_V(2/a)$ ev

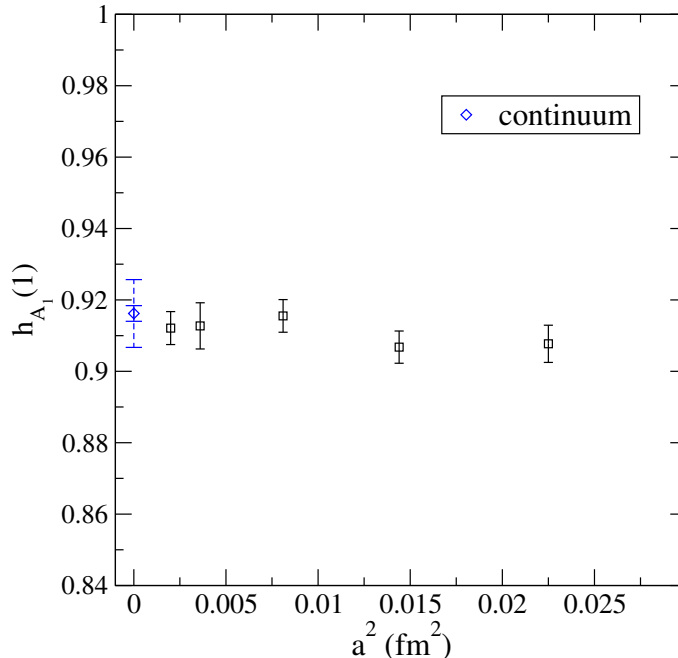


FIG. 7. $h_{A_1}(1)$ versus a^2 for spectator mass $m_x = 0.2m'_s$. The blue point at $a = 0$ shows the extrapolated value for this m_x including the heavy-quark discretization error added in quadrature with the statistical error.

TABLE X. Final error budget for $h_{A_1}(1)$ where each error is discussed in the text. Systematic errors are added in quadrature and combined in quadrature with the statistical error to obtain the total error.

Uncertainty	$h_{A_1}(1)$
Statistics	0.4%
Scale (r_1) error	0.1%
χ PT fits	0.5%
$g_{D^*D\pi}$	0.3%
Discretization errors	1.0%
Perturbation theory	0.4%
Isospin	0.1%
Total	1.4%

G. Isospin Effects

The experimental measurements of the branching fraction for $B \rightarrow D^*\ell\nu$ assume isospin symmetry, and different isospin channels are averaged together [76]. We estimate the size of the effect of isospin corrections based on the chiral extrapolation. One could explicitly include the difference between u and d quark masses in the chiral effective theory, though this has not been worked out through one-loop for this process, to the best of our knowledge. As a simple estimate of the size of isospin effects we vary the end point of our chiral extrapolation between the physical π^+ and the π^0 mass. We use the π^+ mass extrapolation for our central value, but shifting to the π^0 changes the result by 0.1%. Changing the charm mass splitting between the D^{*0} and the D^{*+} is a much smaller effect. Thus, we quote an error of 0.1% due to isospin effects.

VIII. ELECTROWEAK EFFECTS

In this section, we discuss the electroweak and electromagnetic effects in the semileptonic rate, Eq. (1.3). They do not enter the lattice-QCD calculation but are needed, in addition to the hadronic form factor $\mathcal{F}(1) = h_{A_1}(1)$, to obtain $|V_{cb}|$. The factor η_{EW} (written as η_{em} in Ref. [1]) takes the form [10]

$$\eta_{EW} = 1 + \frac{\alpha}{\pi} \left[\ln \frac{M_W}{\mu} + \tan^2 \theta_W \frac{M_W^2}{M_Z^2 - M_W^2} \ln \frac{M_Z}{M_W} \right], \quad (8.1)$$

where the weak mixing angle is specified via $\cos \theta_W = g_2/(g_2^2 + g_1^2)^{1/2}$; g_2 and g_1 are the gauge couplings of $SU(2) \times U(1)$. The first (second) term stems from W -photon (W - Z) box diagrams plus associated parts from vertex and wavefunction renormalization. This form assumes that G_F in Eq. (1.3) is defined via the muon lifetime, which is the case for G_F in Ref. [1]. In the SM, $M_W = M_Z \cos \theta_W$, and the bracket simplifies to $\ln(M_Z/\mu)$. With this assumption, taking the factorization scale $\mu = M_{B^\pm}$, and varying μ by a factor of 2 to estimate the error, one finds

$$\eta_{EW,SM} = 1.00662(16). \quad (8.2)$$

TABLE XI. Values of $|V_{cb}|$ implied by different choices of experimental inputs when accounting for electroweak and Coulomb corrections. The first column is the mode or combination of modes that is taken from experiment, the second and third columns give the experimental value for $10^3|V_{cb}|\bar{\eta}_{EW}\mathcal{F}(1)$ and its source, the fourth column is our estimate of the correction factor $|\bar{\eta}_{EW}|$, the last column is the resulting $10^3|V_{cb}|$ using the result in Eq. (9.1).

Mode	$10^3 V_{cb} \bar{\eta}_{EW}\mathcal{F}(1)$	Ref.	$ \bar{\eta}_{EW} $	$10^3 V_{cb} $
B^0	35.60 ± 0.57	[81]	1.0182 ± 0.0016	$38.59 \pm 0.62_{\text{expt}} \pm 0.52_{\text{QCD}} \pm 0.06_{\text{QED}}$
B^\pm	35.14 ± 1.45	BaBar [82]	1.0066 ± 0.0016	$38.53 \pm 1.60_{\text{expt}} \pm 0.52_{\text{QCD}} \pm 0.06_{\text{QED}}$
Both	40.00 ± 2.04	CLEO [83]	1.0124 ± 0.0058	$43.61 \pm 2.22_{\text{expt}} \pm 0.59_{\text{QCD}} \pm 0.25_{\text{QED}}$
Both	35.83 ± 1.12	BaBar [84]	1.0124 ± 0.0058	$39.06 \pm 1.22_{\text{expt}} \pm 0.53_{\text{QCD}} \pm 0.22_{\text{QED}}$
Both	35.90 ± 0.45	HFAG [76]	1.015 ± 0.005	$39.04 \pm 0.49_{\text{expt}} \pm 0.53_{\text{QCD}} \pm 0.19_{\text{QED}}$

To reiterate, it is theoretically cleaner not to include this factor in $\mathcal{F}(w)$. This way makes it more straightforward to study or remove the μ dependence in future work.

In the experiments [76], the charged-lepton energy spectrum is corrected for bremsstrahlung with the PHOTOS [77] generator. For charged B decay, this package has been shown [78] to reproduce the exact formula [79]. For neutral B decay, the charged D^- and l^+ in the final state attract each other, which is reflected in a slightly different formula for the radiation [11]. Reference [12] recommends treating this effect with a Coulomb correction, $1 + \alpha\pi/2 = 1.01146$ on the amplitude, which is larger than the electroweak correction and similar in size to the uncertainties from experiment and from QCD. Note, however, that a detailed study of radiative corrections in $K \rightarrow \pi l \nu$ finds that QCD-scale effects reduce the Coulomb effects, such that the total is closer to 1% than 2% [80]. Already now, and certainly for any future determination of $|V_{cb}|$, a similar treatment is called for, theoretically first and then in the combination of experimental measurements of neutral and charged decays.

The current experiments do not take the Sirlin [10] and Coulomb effects into account. Further, to our knowledge a study of QCD-scale photons, analogous to Ref. [80], is not available for heavy-meson decays. In particular, charged and neutral decays are analyzed and combined without different radiative corrections. The quantity reported to be $|V_{cb}|\mathcal{F}(1)$ is really $|V_{cb}|\bar{\eta}_{EW}\mathcal{F}(1)$, where $\bar{\eta}_{EW}$ is a suitably charge-weighted average of Eq. (8.1) and the Coulomb effect. Table XI shows results for $|V_{cb}|$ from different choices for the experimental input and the corresponding estimate of $\bar{\eta}_{EW}$. The first entry shows an average with HFAG methods from B^0 decays only [81], while the second shows the B^\pm -only measurement from BaBar [82]; then $\bar{\eta}_{EW}$ is simply Eq. (8.2) with and without the Coulomb factor, respectively. The third and fourth entries are the results from single experiments, CLEO [83] and BaBar [84], in which both modes were combined; here, we compute $\bar{\eta}_{EW}$ by assuming a 50-50 split, varying between 100-0 and 0-100 to estimate the error. This range is extreme, but with one experiment, the QCD and QED errors are smaller than the experimental error. The last row in Table XI shows the 2012 result from HFAG [76] with our estimate of the appropriate charge-weighted average for $\bar{\eta}_{EW}$. The neutral data carry greater weight in the HFAG average [81], so we take a value of $\bar{\eta}_{EW}$ slightly larger than a 50-50 split, with generous error range, to allow for other effects, such as photons at the QCD scale.

IX. RESULTS AND CONCLUSIONS

We have improved on our previous calculation of the zero-recoil form factor for $B \rightarrow D^* \ell \nu$ decay by increasing statistics, going to lighter quark masses at correspondingly larger volumes, and going to finer lattice spacings. Our final result, given the error budget in Table X, is

$$\mathcal{F}(1) = h_{A_1}(1) = 0.906(4)(1)(5)(3)(9)(4)(1), \quad (9.1)$$

where the errors are statistical, scale uncertainty, chiral extrapolation errors, parametric uncertainty in $g_{D^*D\pi}$, heavy-quark discretization errors, perturbative matching, and isospin effects. Adding all systematic errors in quadrature, we obtain $h_{A_1}(1) = 0.906(4)(12)$, which is consistent with our previous published result $h_{A_1}(1) = 0.921(13)(20)$ [7], but with a significantly smaller error. The data added since our preliminary report [8] have reduced the χ PT and $g_{D^*D\pi}$ errors moderately.

From Table XI, we choose the HFAG average of all data, with our conservative estimate of the QED correction, as our preferred way of obtaining $|V_{cb}|$. Thus, we find

$$|V_{cb}| = (39.04 \pm 0.49_{\text{expt}} \pm 0.53_{\text{QCD}} \pm 0.19_{\text{QED}}) \times 10^{-3}. \quad (9.2)$$

The QCD error is now commensurate with the experimental error. This result is in agreement with our previous published result [7], but differs by 3.0σ from the inclusive determination $|V_{cb}| = (42.42 \pm 0.86) \times 10^{-3}$ [85].

The largest error in our determination of $h_{A_1}(1)$ is the systematic error due to heavy-quark discretization effects. We have made a detailed study of the expected a dependence using HQET at finite lattice spacing. A value of $\bar{\Lambda}$ is needed to compute this dependence; our choice of $\bar{\Lambda} \approx 450$ MeV is consistent with the size of the discretization effects seen in the numerical data and can reproduce the behavior of these effects over the five lattice spacings included in our calculation. We could reduce this error by going to finer lattice spacings or by using a more improved Fermilab action, *e.g.*, the Oktay-Kronfeld action [86]. When using this action, it would be necessary to improve the currents to the same order.

Several subleading errors appear in our calculation at the 0.4-0.6% level. They would be nontrivial to improve. Reducing the error from the QED Coulomb correction would require a detailed study of electromagnetic effects within HQET, and reducing the QCD matching error would require a two-loop lattice perturbation theory calculation or nonperturbative matching. The chiral extrapolation error would not necessarily be reduced by a straightforward simulation at the physical light-quark masses because the D^* would become unstable apart from finite-volume effects. At the current level of precision, it is important to extend the calculation to nonzero recoil. This would provide a useful cross-check of the method used to extrapolate the experimental form factor to zero recoil [87]. Another important cross-check is our companion calculation of $|V_{cb}|$ using the $B \rightarrow D \ell \nu$ decay, has been reported in Ref. [88]. Full details, including its determination of $|V_{cb}|$, will be presented in a forthcoming paper.

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Appendix A: Staggered Chiral Perturbation Theory for $B \rightarrow D^* \ell \nu$ at zero-recoil

The partially quenched expression for h_{A_1}/η_A at zero-recoil through NLO in staggered chiral perturbation theory was derived in Ref. [64]. For completeness, it is given here. The result is

$$\begin{aligned}
\frac{h_{A_1}^{(B_x)PQ,2+1}(1)}{\eta_A} &= 1 + \frac{X_A(\Lambda_\chi)}{m_c^2} + \frac{g_{DD^*\pi}^2}{48\pi^2 f^2} \left\{ \frac{1}{16} \sum_{\substack{j=xu,xu,xs \\ \Xi=I,P,4V,4A,6T}} \bar{F}_{j\Xi} \right. \\
&+ \frac{1}{3} \left[R_{X_I}^{[2,2]}(\{M_{X_I}^{(5)}\}; \{\mu_I\}) \left(\frac{d\bar{F}_{X_I}}{dM_{X_I}^2} \right) - \sum_{j \in \{M_I^{(5)}\}} D_{j,X_I}^{[2,2]}(\{M_{X_I}^{(5)}\}; \{\mu_I\}) \bar{F}_j \right] \\
&+ a^2 \delta'_V \left[R_{X_V}^{[3,2]}(\{M_{X_V}^{(7)}\}; \{\mu_V\}) \left(\frac{d\bar{F}_{X_V}}{dM_{X_V}^2} \right) - \sum_{j \in \{M_V^{(7)}\}} D_{j,X_V}^{[3,2]}(\{M_{X_V}^{(7)}\}; \{\mu_V\}) \bar{F}_j \right] \\
&\left. + (V \rightarrow A) \right\}, \tag{A1}
\end{aligned}$$

where

$$\begin{aligned}
F(M_j, z_j) &= \frac{M_j^2}{z_j} \left\{ z_j^3 \ln \frac{M_j^2}{\Lambda_\chi^2} - \frac{2}{3} z_j^3 - 4z_j + 2\pi \right. \\
&\quad \left. - \sqrt{z_j^2 - 1} (z_j^2 + 2) \left(\ln \left[1 - 2z_j(z_j - \sqrt{z_j^2 - 1}) \right] - i\pi \right) \right\} \\
&\rightarrow (\Delta^{(c)})^2 \ln \left(\frac{M_j^2}{\Lambda_\chi^2} \right) + \mathcal{O}[(\Delta^{(c)})^3],
\end{aligned} \tag{A2}$$

with $\bar{F}(M_j, z_j) = F(M_j, -z_j)$, and $z_j = \Delta^{(c)}/M_j$, where $\Delta^{(c)}$ is the D - D^* mass splitting. The residues $R_j^{[n,k]}$ and $D_{j,i}^{[n,k]}$ are defined in Refs. [89, 90]. These residues are a function of two sets of masses, the numerator masses, $\{M\} = \{M_1, M_2, \dots, M_n\}$ and the denominator masses, $\{\mu\} = \{\mu_1, \mu_2, \dots, \mu_k\}$. In our 2+1 flavor case, we have

$$\begin{aligned}
\{M_X^{(5)}\} &\equiv \{M_\eta, M_X\}, \\
\{M_X^{(7)}\} &\equiv \{M_\eta, M_{\eta'}, M_X\}, \\
\{\mu\} &\equiv \{M_U, M_S\}.
\end{aligned} \tag{A3}$$

The expressions for the masses $M_{\eta'}$, M_{η_V} , $M_{\eta'_V}$ in terms of the parameters of the rooted staggered effective theory are given in Ref. [89].

Appendix B: Heavy-quark Discretization Effects

Let us define the various discretization errors in $\rho_{Aj} \sqrt{R_{A_1}}$ via

$$\rho_{Aj} \sqrt{R_{A_1}} = h_{A_1}(1) + \mathcal{O}(\alpha_s^{1+\ell_\rho}) + \mathcal{O}(\alpha_s^{1+\ell_c} a \bar{\Lambda}^2 / m_c) + \mathcal{O}(\alpha_s^{1+\ell_d} a^2 \bar{\Lambda}^2), \tag{B1}$$

where $\bar{\Lambda} \approx M_B - m_b$ is a measure of nonperturbative QCD effects in heavy-light mesons. These stem, respectively, from the truncation of the perturbative series for ρ_{Aj} , truncation of the perturbative series for c_{SW} (*i.e.*, improvement of the action), and from mismatches in the improved lattice currents. That the power-law effects in Eq. (B1) start with $\bar{\Lambda}^2$ is a special property of zero recoil, established below. As written, Eq. (B1) holds for general, multi-loop matching; for the calculation described in this paper, we have one-loop matching for ρ_{Aj} , so $\ell_\rho = 1$, and we have tree-level improvement for the action and current, so $\ell_c = \ell_d = 0$.

We now assemble the formulae needed to prove the appearance of $\bar{\Lambda}^2$. The discretization effects are estimated with the heavy-quark effective field theory (HQET) [53, 54]. Wilson fermions exhibit heavy-quark symmetries for small κ , so HQET provides a suitable description. For the lattice gauge theory (LGT) Lagrangian,

$$\mathcal{L}_{\text{LGT}} \doteq \bar{h}(iv \cdot D - m_1)h + \frac{\bar{h}D_\perp^2 h}{2m_2} + \frac{\bar{h}s \cdot Bh}{2m_B} + \frac{\bar{h}[D_\perp^\alpha, iE_\alpha]h}{8m_D^2} + \frac{\bar{h}s_{\alpha\beta}\{D_\perp^\alpha, iE^\beta\}h}{4m_E^2} + \dots, \tag{B2}$$

where \doteq can be read “has the same matrix elements as.” Here, v is a four vector specifying the rest-frame of the heavy-light meson, such that $v^2 = -1$; the heavy-quark field h satisfies $-i\not{v}h = h$, and $s_{\alpha\beta} = -i\sigma_{\alpha\beta}/2$. Then, $D_\perp^\mu = D^\mu + v^\mu v \cdot D$ is the covariant derivative orthogonal to v , $B^{\alpha\beta} = (\delta_\mu^\alpha + v^\alpha v_\mu)F^{\mu\nu}(\delta_\nu^\beta + v^\beta v_\nu)$ is the chromomagnetic field (in the

v frame), and $E^\beta = -v_\alpha F^{\alpha\beta}$ is the chromoelectric field (in the v frame). The HQET description for continuum QCD has the same structure

$$\mathcal{L}_{\text{QCD}} \doteq \bar{h}(iv \cdot D - m)h + \frac{\bar{h}D_\perp^2 h}{2m} + \frac{z_B \bar{h}s \cdot Bh}{2m} + \frac{z_D \bar{h}[D_\perp^\alpha, iE_\alpha]h}{8m^2} + \frac{z_E \bar{h}s_{\alpha\beta}\{D_\perp^\alpha, iE^\beta\}h}{4m^2} + \dots \quad (\text{B3})$$

In matrix elements, the rest mass m_1 does not enter, so one tunes κ so that

$$\frac{1}{2m_2} = \frac{1}{2m}, \quad (\text{B4})$$

and c_{SW} so that

$$\frac{1}{2m_B} = \frac{z_B}{2m} = \frac{1 + \text{O}(\alpha_s)}{2m}, \quad (\text{B5})$$

where the second equality follows because $z_B = 1 + \text{O}(\alpha_s)$. In practice, we tune κ via the heavy-strange *meson* mass, as discussed in Appendix C, and we choose c_{SW} at the tadpole-improved tree level, which brings in the second error exhibited in Eq. (B1).

The LGT currents can also be described in the HQET, and the full description entails many operators [53, 54]. Here, however, we need only the temporal vector current:

$$\begin{aligned} Z_{V_{cb}} V^4 = -Z_{V_{cb}} v \cdot V &\doteq \bar{C}_{V_{cb}} \bar{c}b + \eta_{V_{cb}D_\perp^2}^{(0,2)} \frac{\bar{c}D_\perp^2 b}{8m_{D_\perp^2 b}^2} + \eta_{V_{cb}sB}^{(0,2)} \frac{\bar{c}s \cdot Bb}{8m_{sB}^2} - \eta_{V_{cb}\alpha E}^{(0,2)} \frac{\bar{c}i\not{E}b}{4m_{\alpha Eb}^2} \\ &+ \eta_{V_{cb}D_\perp^2}^{(2,0)} \frac{\overleftarrow{c}D_\perp^2 b}{8m_{D_\perp^2 c}^2} + \eta_{V_{cb}sB}^{(2,0)} \frac{\bar{c}s \cdot Bb}{8m_{sBc}^2} + \eta_{V_{cb}\alpha E}^{(2,0)} \frac{\bar{c}i\not{E}b}{4m_{\alpha Ec}^2} \\ &+ z_{V_{cb}1}^{(1,1)} \frac{\overleftarrow{c}D_\perp \cdot D_\perp b}{2m_{3c} 2m_{3b}} + z_{V_{cb}s}^{(1,1)} \frac{\overleftarrow{c}D_\perp^\alpha s_{\alpha\beta} D_\perp^\beta b}{2m_{3c} 2m_{3b}}, \end{aligned} \quad (\text{B6})$$

and the spatial axial vector current (ϵ is the D^* polarization vector):

$$\begin{aligned} Z_{A_{cb}} \epsilon \cdot A &\doteq \bar{C}_{A_{cb}} \bar{c}\not{\epsilon}_\perp \gamma^5 b + \eta_{A_{cb}D_\perp^2}^{(0,2)} \frac{\bar{c}\not{\epsilon}_\perp \gamma^5 D_\perp^2 b}{8m_{D_\perp^2 b}^2} + \eta_{A_{cb}sB}^{(0,2)} \frac{\bar{c}\not{\epsilon}_\perp \gamma^5 s \cdot Bb}{8m_{sB}^2} - \eta_{A_{cb}\alpha E}^{(0,2)} \frac{\bar{c}\not{\epsilon}_\perp \gamma^5 i\not{E}b}{4m_{\alpha Eb}^2} \\ &+ \eta_{A_{cb}D_\perp^2}^{(2,0)} \frac{\overleftarrow{c}D_\perp^2 \not{\epsilon}_\perp \gamma^5 b}{8m_{D_\perp^2 c}^2} + \eta_{A_{cb}sB}^{(2,0)} \frac{\bar{c}s \cdot B\not{\epsilon}_\perp \gamma^5 b}{8m_{sBc}^2} + \eta_{A_{cb}\alpha E}^{(2,0)} \frac{\bar{c}i\not{E}\not{\epsilon}_\perp \gamma^5 b}{4m_{\alpha Ec}^2} \\ &+ z_{A_{cb}1}^{(1,1)} \frac{\overleftarrow{c}(\not{D}_\perp \not{\epsilon}_\perp \gamma^5 D_\perp)_1 b}{2m_{3c} 2m_{3b}} + z_{A_{cb}s}^{(1,1)} \frac{\overleftarrow{c}(\not{D}_\perp \not{\epsilon}_\perp \gamma^5 D_\perp)_s b}{2m_{3c} 2m_{3b}}. \end{aligned} \quad (\text{B7})$$

The continuum currents enjoy the same description, but with different short-distance coefficients. The matching factors Z_V and Z_A are defined so that the leading operators on the right-hand sides of Eqs. (B6) and (B7) share the normalization with the corresponding continuum currents. With the one-loop calculation of ρ_{Aj} , explained in Sec. IV, the matching leads to $\ell_\rho = 1$ in Eq. (B1). For the currents defined in Sec. II B, as well as for the continuum currents, the η -coefficients and z -coefficients all take the form $1 + \text{O}(\alpha_s)$. The rotation in Eq. (2.8) ensures that

$$\frac{1}{2m_3} = \frac{1}{2m_2} + \text{O}(\alpha_s a), \quad (\text{B8})$$

i.e., $\ell_d = 0$ in Eq. (B1). The other masses in Eqs. (B6) and (B7) deviate from m_2 when $m_2 a \not\ll 1$ but all collapse to m_2 as $m_2 a \rightarrow 0$ [47, 86]. These properties of the coefficients are crucial to the proof that the discretization effects start with $\bar{\Lambda}^2$ in Eq. (B1).

Note that no dimension-four currents arise, which would describe discretization errors starting at order $a\bar{\Lambda}$. At nonzero recoil, such currents do appear, and their discretization errors are shown in detail in Eqs. (2.37)–(2.44) of Ref. [54]. At zero recoil, the heavy-quark symmetry enlarges from $\text{SU}_{b\text{-spin}}(2) \times \text{SU}_{c\text{-spin}}(2)$ to $\text{SU}_{\text{spin-flavor}}(4)$, and a generalization of Luke’s theorem requires the leading discretization/heavy-quark effects to vanish. The discretization effects then stem from second-order breaking of heavy-quark symmetry, as explained in Ref. [53], leading to the extra suppression of $\bar{\Lambda}/m_c$ or $a\bar{\Lambda}$ in Eq. (B1). Luke’s theorem also ensures that single insertions of chromoelectric interactions (spin-orbit and Darwin terms) drop out at zero recoil.

We proceed by collecting results from Ref. [53] for the zero-recoil discretization errors in matrix elements of the currents in Eqs. (2.6) and (2.7) and combining them into a formula for the discretization error in $\rho_{Aj} \sqrt{R_{A_1}}$. (Note that in Ref. [53] $\rho_A \sqrt{R_{A_1}}$ stands for a different double ratio.) The discretization errors stem from all higher-dimension terms on the right-hand sides of Eqs. (B2), (B6), and (B7), but always take the form

$$\text{error}_i = \left(\mathcal{C}_i^{\text{LGT}} - \mathcal{C}_i^{\text{QCD}} \right) \langle \mathcal{O}_i \rangle, \quad (\text{B9})$$

where the \mathcal{C}_i denote the short-distance coefficients, which are different for the lattice and continuum, and the \mathcal{O}_i denotes the HQET operators on the right-hand sides of Eqs. (B2), (B6), and (B7). To get the errors, we then combine asymptotic forms of $\mathcal{C}_i^{\text{LGT}} - \mathcal{C}_i^{\text{QCD}}$ with power-counting estimates of $\langle \mathcal{O}_i \rangle$. The former have been derived in Refs. [47, 86], and the latter are guided by the data and some theoretical considerations to arrive at concrete error estimates.

1. Second-order formulas at zero recoil

From Eqs. (7.20) and (7.30) of Ref. [53], the HQET expansions through $\text{O}(\bar{\Lambda}^2)$ of the matrix elements are

$$\langle B | Z_{V_{bb}^4} V^4 | B \rangle = 1 + W_{00}^{(2)}, \quad (\text{B10})$$

$$\langle D^*(\boldsymbol{\epsilon}) | Z_{V_{cc}^4} V^4 | D^*(\boldsymbol{\epsilon}) \rangle = 1 + W_{11}^{(2)}, \quad (\text{B11})$$

$$\langle D^*(\boldsymbol{\epsilon}) | Z_{A_{cb}^i} \boldsymbol{\epsilon} \cdot \mathbf{A} | B \rangle = \bar{C}_{A_{\perp}^{cb}} W_{01}^{(0)} + W_{01}^{(2)}, \quad (\text{B12})$$

where $\bar{C}_{A_{\perp}^{cb}} = 1 + \text{O}(\alpha_s)$ is a short-distance coefficient in Eq. (B7), and $W_{01}^{(2)}$ is written $\bar{W}_{01}^{(2)} + \delta W_{01}^{(2)}$ in Ref. [53]. The subscripts on $W_{JJ'}^{(i)}$ indicate the meson spins ($J = 0$ for B and $J = 1$ for D^*), and the superscript denotes the order in the heavy-quark expansion of the currents. The expressions for the vector-current matrix elements have been simplified by noting $\bar{C}_{V_{\parallel}^{hh}} = 1$ for the flavor-diagonal vector current, and $W_{JJ}^{(0)} = 1$ for $h \rightarrow h$ transitions. Combining Eqs. (B10)–(B12), one finds the $\text{O}(\bar{\Lambda}^2)$ expansion

$$\rho_{Aj} \sqrt{R_{A_1}} = \bar{C}_{A_{\perp}^{cb}} W_{01}^{(0)} + W_{01}^{(2)} - \frac{1}{2} \bar{C}_{A_{\perp}^{cb}} \left(W_{00}^{(2)} + W_{11}^{(2)} \right). \quad (\text{B13})$$

We must obtain more explicit expressions for the terms on the right-hand side and compare them to the analogous terms in the HQET expansion of $h_{A_1}(1)$ in continuum QCD.

Let us start with $W_{01}^{(0)}$. From Eq. (7.31) of Ref. [53]

$$W_{01}^{(0)} = 1 - \frac{1}{2}\Delta_2(\Delta_2 D - 2\Theta_B E) - \frac{1}{2}\Delta_B(\Delta_B R_1 - \Theta_B R_2) - \frac{1}{2m_{Bc}2m_{Bb}}\left(\frac{4}{3}R_1 + 2R_2\right), \quad (\text{B14})$$

where D , E , R_1 , and R_2 are HQET matrix elements of order $\bar{\Lambda}^2$, and

$$\Delta_I = \frac{1}{2m_{Ic}} - \frac{1}{2m_{Ib}}, \quad I = 2, B, \quad (\text{B15})$$

$$\Theta_I = \frac{1}{2m_{Ic}} + \frac{3}{2m_{Ib}} \quad (\text{B16})$$

are combinations of the mass coefficients in Eq. (B2). Beyond the leading 1, the terms in $W_{01}^{(0)}$ come from double insertions of the kinetic and chromomagnetic interactions. Equation (B14) makes clear that we are working through $\mathcal{O}(\bar{\Lambda}^2)$ in the heavy-quark expansion, although it accommodates, in principle, all orders in perturbation theory in α_s .

To obtain the analogous expression for Eq. (B14) in continuum QCD, simply replace $m_{2h} \rightarrow m_h$ (because that is how the hopping parameter is tuned in the Fermilab method) and $1/m_{Bh} \rightarrow z_B/m_h$ [compare Eqs. (B2) and (B3)]. Taking the difference, one sees that the error in $W_{01}^{(0)}$ stems from

$$\frac{1}{2m_{Bh}} - \frac{z_B}{2m_{2h}} = af_{Bh}. \quad (\text{B17})$$

We have chosen c_{SW} such that f_{Bh} is of order α_s , and the mismatches in $W_{01}^{(0)}$ lead to errors of order $\alpha_s a \bar{\Lambda}^2/m_h$.

Now let us turn to the error in the other terms in Eq. (B13) and combine them into

$$\ddot{W}_{01}^{(2)} = W_{01}^{(2)} - \frac{1}{2}\bar{C}_{A_\perp^{cb}} \left(W_{00}^{(2)} + W_{11}^{(2)} \right). \quad (\text{B18})$$

The right-hand side comes from the matrix elements of the dimension-five terms in Eqs. (B6) and (B7). The matrix elements of \not{E} vanish, and the others lead to

$$W_{JJ}^{(2)} = - \left(\frac{1}{4m_{D_\perp^2 h}^2} - \frac{z_{V^{hh_1}}^{(1,1)}}{(2m_{3h})^2} \right) \mu_\pi^2 + d_J \left(\frac{1}{4m_{sBh}^2} - \frac{z_{V^{hh_s}}^{(1,1)}}{(2m_{3h})^2} \right) \frac{\mu_G^2}{3}, \quad (\text{B19})$$

$$\begin{aligned} W_{01}^{(2)} = & - \left(\frac{\eta_{A^{cb}D_\perp^2}^{(2,0)}}{8m_{D_\perp^2 c}^2} + \frac{\eta_{A^{cb}D_\perp^2}^{(0,2)}}{8m_{D_\perp^2 b}^2} + \frac{1}{3} \frac{z_{A^{cb1}}^{(1,1)}}{2m_{3c}2m_{3b}} \right) \mu_\pi^2 \\ & - \left(\frac{\eta_{A^{cb_sB}}^{(2,0)}}{8m_{sBc}^2} - \frac{\eta_{A^{cb_sB}}^{(0,2)}}{8m_{sBb}^2} - \frac{z_{A^{cb_s}}^{(1,1)}}{2m_{3c}2m_{3b}} \right) \frac{\mu_G^2}{3}, \end{aligned} \quad (\text{B20})$$

as in Eqs. (7.22), (7.33) and (7.34) of Ref. [53]. Here, μ_π^2 is the heavy-quark kinetic energy, and μ_G^2 is known from the B^*-B splitting. Both μ_π^2 and μ_G^2 are of order $\bar{\Lambda}^2$. (Ref. [53] used another notation with $\mu_\pi^2 = -\lambda_1$ and $\mu_G^2 = 3\lambda_2$.) We choose to define $m_{D_\perp^2 h}^2$ and m_{sBh}^2 to all orders in α_s via the degenerate-mass vector current, so $\eta_{V^{hh}D_\perp^2}^{(2,0)} \equiv 1$, etc., so no η -like coefficients appear in Eq. (B19).

At the tree level, the coefficients written as inverse masses are the same for all currents. By construction, $\eta_{A^{cb}D_{\perp}^2}^{(2,0)}$, $\eta_{A^{cb}D_{\perp}^2}^{(0,2)}$, $\eta_{A^{cb}sB}^{(2,0)}$, and $\eta_{A^{cb}sB}^{(0,2)}$ take the form $1 + \mathcal{O}(\alpha_s)$. Furthermore, an analogous all-orders definition of m_{3h} ensures that the $z_{J_{\bullet}}^{(1,1)}$ take the form $1 + \mathcal{O}(\alpha_s)$ too. As $a \rightarrow 0$, the right-hand sides of Eqs. (B19) and (B20) approach continuum QCD. In particular, the quantities inside large parentheses in Eq. (B19) must vanish as $a \rightarrow 0$.

Combining Eqs. (B19) and (B20) as specified in Eq. (B18),

$$\begin{aligned} \ddot{W}_{01}^{(2)} = & - \left(\frac{\eta_{A^{cb}D_{\perp}^2}^{(2,0)} - \bar{C}_{A_{\perp}^{cb}}}{8m_{D_{\perp}^2 c}^2} + \frac{\bar{C}_{A_{\perp}^{cb}} z_{V^{cc1}}^{(1,1)}}{8m_{3c}^2} + \frac{\eta_{A^{cb}D_{\perp}^2}^{(0,2)} - \bar{C}_{A_{\perp}^{cb}}}{8m_{D_{\perp}^2 b}^2} + \frac{\bar{C}_{A_{\perp}^{cb}} z_{V^{bb1}}^{(1,1)}}{8m_{3b}^2} + \frac{z_{A^{cb1}}^{(1,1)}}{3 \cdot 2m_{3c} 2m_{3b}} \right) \mu_{\pi}^2 \\ & - \left(\frac{\eta_{A^{cb}sB}^{(2,0)} - \bar{C}_{A_{\perp}^{cb}}}{8m_{sBc}^2} + \frac{\bar{C}_{A_{\perp}^{cb}} z_{V^{ccs}}^{(1,1)}}{8m_{3c}^2} - 3 \frac{\eta_{A^{cb}sB}^{(0,2)} - \bar{C}_{A_{\perp}^{cb}}}{8m_{sBb}^2} - 3 \frac{\bar{C}_{A_{\perp}^{cb}} z_{V^{bbs}}^{(1,1)}}{8m_{3b}^2} - \frac{z_{A^{cb}s}^{(1,1)}}{2m_{3c} 2m_{3b}} \right) \frac{\mu_G^2}{3}, \end{aligned} \quad (\text{B21})$$

Once again, the analogous expression in continuum QCD can be obtained from $\ddot{W}_{01}^{(2)}$ by changing the short-distance coefficients accordingly. The errors in $\ddot{W}_{01}^{(2)}$ stem from the mismatches

$$a^2 f_{D_{\perp}^2 c} = \frac{\eta_{A^{cb}D_{\perp}^2}^{(2,0)}(m_{0c}a, m_{0b}a)}{8m_{D_{\perp}^2 c}^2} - \frac{\bar{C}_{A_{\perp}^{cb}}}{8m_{D_{\perp}^2 c}^2} + \frac{\bar{C}_{A_{\perp}^{cb}} z_{V^{cc1}}^{(1,1)}(m_{0c}a, m_{0b}a)}{8m_{3c}^2} - \frac{\eta_{A^{cb}D_{\perp}^2}^{(2,0)}(m_c/m_b)}{8m_{2c}^2}, \quad (\text{B22})$$

$$a^2 f_{D_{\perp}^2 b} = \frac{\eta_{A^{cb}D_{\perp}^2}^{(0,2)}(m_{0c}a, m_{0b}a)}{8m_{D_{\perp}^2 b}^2} - \frac{\bar{C}_{A_{\perp}^{cb}}}{8m_{D_{\perp}^2 b}^2} + \frac{\bar{C}_{A_{\perp}^{cb}} z_{V^{bb1}}^{(1,1)}(m_{0c}a, m_{0b}a)}{8m_{3b}^2} - \frac{\eta_{A^{cb}D_{\perp}^2}^{(0,2)}(m_c/m_b)}{8m_{2b}^2}, \quad (\text{B23})$$

$$a^2 f_{sBc} = \frac{\eta_{A^{cb}sB}^{(2,0)}(m_{0c}a, m_{0b}a)}{8m_{sBc}^2} - \frac{\bar{C}_{A_{\perp}^{cb}}}{8m_{sBc}^2} + \frac{\bar{C}_{A_{\perp}^{cb}} z_{V^{ccs}}^{(1,1)}(m_{0c}a, m_{0b}a)}{8m_{3c}^2} - \frac{\eta_{A^{cb}sB}^{(2,0)}(m_c/m_b)}{8m_{2c}^2}, \quad (\text{B24})$$

$$a^2 f_{sBb} = \frac{\eta_{A^{cb}sB}^{(0,2)}(m_{0c}a, m_{0b}a)}{8m_{sBb}^2} - \frac{\bar{C}_{A_{\perp}^{cb}}}{8m_{sBb}^2} + \frac{\bar{C}_{A_{\perp}^{cb}} z_{V^{bbs}}^{(1,1)}(m_{0c}a, m_{0b}a)}{8m_{3b}^2} - \frac{\eta_{A^{cb}sB}^{(0,2)}(m_c/m_b)}{8m_{2b}^2}, \quad (\text{B25})$$

$$a^2 f_{3c3b1} = \frac{z_{A^{cb1}}^{(1,1)}(m_{0c}a, m_{0b}a)}{2m_{3c} 2m_{3b}} - \frac{z_{A^{cb1}}^{(1,1)}(m_c/m_b)}{2m_{2c} 2m_{2b}}, \quad (\text{B26})$$

$$a^2 f_{3c3bs} = \frac{z_{A^{cb}s}^{(1,1)}(m_{0c}a, m_{0b}a)}{2m_{3c} 2m_{3b}} - \frac{z_{A^{cb}s}^{(1,1)}(m_c/m_b)}{2m_{2c} 2m_{2b}}, \quad (\text{B27})$$

where the right-most terms are those stemming from continuum QCD. Because the Fermilab method is based on Wilson fermions (as opposed to lattice NRQCD), the continuum limit of the η s and z s must tend as $a \rightarrow 0$ to the analogous coefficients for continuum QCD:

$$\lim_{a \rightarrow 0} \eta_{J_{\bullet}}^{(\bullet)}(m_{0c}a, m_{0b}a) = \eta_{J_{\bullet}}^{(\bullet)}(m_c/m_b) \quad (\text{B28})$$

$$\lim_{a \rightarrow 0} z_{J_{\bullet}}^{(1,1)}(m_{0c}a, m_{0b}a) = z_{J_{\bullet}}^{(1,1)}(m_c/m_b) \quad (\text{B29})$$

with $m_c/m_b = m_{0c}a/m_{0b}a$ fixed. Therefore, in Eqs. (B22)–(B25), the first and fourth should cancel against each other, and so should the second and third. At nonzero lattice spacing, even when $m_{0h}a \sim 1$, the difference between the first and second terms is of order α_s , and similarly for the difference between the third and fourth terms. This complicated pattern of cancellation ensures that the right-hand sides of Eqs. (B22)–(B25) is of order $\alpha_s a^2$. Similarly,

the cancellation on the right-hand sides of Eqs. (B26) and (B27) also leaves mismatches of order $\alpha_s a^2$.

This completes the demonstration that the heavy-quark discretization effects in Eq. (B1) start with $\bar{\Lambda}^2$. Note especially that the discretization effects of order a from the clover term mistuning are suppressed by an additional (small) factor $\bar{\Lambda}/m_h$. The discretization errors from the currents are, owing to the double-ratio, of order a^2 . Note that to extend Eq. (B1) beyond $\ell_d = 0$, we would need not only one-loop matching of the rotation in Eq. (2.8) but further rotations of the form $D_\perp^2 \psi$ and $sB\psi$. In practice, we have $\ell_d = 0$, so this complication is not needed for now.

2. Discretization errors

We now turn to explicit estimates of the total discretization error. Each term of Eq. (B1) introduces an error into our calculation, which we address in turn. The error of order α_s^2 from the one-loop computation of the matching factor ρ_{Aj} is discussed in Sec. VII F.

a. Errors of order $\alpha_s a \bar{\Lambda}^2 / m_h$

This discretization error stems from the one-loop mismatch of the chromomagnetic masses $1/2m_{Bh}$ appearing in $W_{01}^{(0)}$. From Eq. (B14), it is

$$\begin{aligned} \text{error}_B &= a \frac{f_{Bb}}{2m_{2c}} 4E - a \frac{f_{Bc}}{2m_{2c}} [R_1 - (R_2 + E)] \\ &\quad - \frac{a}{3} \left[\frac{f_{Bb}}{2m_{2c}} + \frac{f_{Bc} + 3f_{Bb}}{2m_{2b}} \right] [R_1 + 3(R_2 + E)], \end{aligned} \quad (\text{B30})$$

where $f_{Bh} = f_B(m_{0h}a)$ is the mismatch function for heavy quark h . The reason for grouping the HQET matrix elements this way is explained below. The mismatch function $f_B(m_0a)$ starts at order α_s , and we do not have an explicit expression for it. (The calculation is what one needs to match c_{SW} at the one-loop level.) We shall take unimproved tree-level coefficients as a guide to the combinatoric factors, leading to the Ansatz

$$f_B(m_0a) = \frac{\alpha_s}{2(1 + m_0a)}. \quad (\text{B31})$$

The relative signs in Eq. (B30) are meaningful once one has chosen a coherent Ansatz for the mass dependence of f_B , such as Eq. (B31), and if, as argued in Sec. B 2 c, we know the relative signs of the HQET matrix elements E , $R_1 - (R_2 + E)$, and $R_1 + 3(R_2 + E)$. If we assume nothing about the latter, then the three terms on the right-hand side of Eq. (B30) should be treated as independent and added in quadrature.

b. Errors of order $\alpha_s a^2 \bar{\Lambda}^2$

These discretization errors stem from the differences in Eqs. (B22)–(B27). Let us start with the first two terms in Eqs. (B22)–(B25). The numerator differences are of order α_s and

the denominators can be deduced from Eqs. (A17) and (A19) of Ref. [47]. When $c_B = r_s$ they share the same coefficient

$$\frac{1}{8m_{D_1^2}^2} = \frac{1}{8m_{sB}^2} = \frac{1}{8m_2^2} + a^2 f_X(m_0 a), \quad (\text{B32})$$

where [47, 86]

$$f_X(m_0 a) = \frac{1}{4(1 + m_0 a)} - \frac{1}{2} \left(\frac{m_0 a}{2(2 + m_0 a)(1 + m_0 a)} \right)^2. \quad (\text{B33})$$

These errors can thus be estimated to be

$$\begin{aligned} \mathbf{error}_{X_1} = & \alpha_s \left[\frac{1}{2(2m_{2c})^2} + a^2 f_{Xc} + \frac{1}{2(2m_{2b})^2} + a^2 f_{Xb} \right] \mu_\pi^2 \\ & + \alpha_s \left[\frac{1}{3} \frac{1}{2(2m_{2c})^2} + a^2 \frac{1}{3} f_{Xc} - \frac{1}{2(2m_{2b})^2} - a^2 f_{Xb} \right] \mu_G^2 \end{aligned} \quad (\text{B34})$$

where the relative signs and combinatorial factors have been retained. We do not, however, know the sign and size of the (omitted) one-loop coefficients multiplying the two brackets. In Eq. (B34), f_{Xh} means to evaluate Eq. (B32) with the $m_0 a$ of quark $h = c, b$.

In Eqs. (B22)–(B25), the cancellation of the third and fourth terms lead to discretization effects correlated with the right-hand side of Eq. (B34). Because the tree-level matches exactly, we have

$$\mathbf{error}_{X_2} = \alpha_s \left[\frac{1}{2(2m_{2c})^2} + \frac{1}{2(2m_{2b})^2} \right] \mu_\pi^2 + \alpha_s \left[\frac{1}{3} \frac{1}{2(2m_{2c})^2} - \frac{1}{2(2m_{2b})^2} \right] \mu_G^2 \quad (\text{B35})$$

As $a \rightarrow 0$, however, \mathbf{error}_{X_2} has to cancel the $1/(2m_2 a)^2$ parts of \mathbf{error}_{X_1} . On the other hand, for $m_0 a \gg 1$, the f_X terms dominate all others. It seems safe, therefore, to combine these errors into

$$\mathbf{error}_X = \alpha_s a^2 (f_{Xc} + f_{Xb}) \mu_\pi^2 + \alpha_s a^2 \left(\frac{1}{3} f_{Xc} - f_{Xb} \right) \mu_G^2. \quad (\text{B36})$$

Here, the relative sign and size of the two terms is unknown, owing to the unknown one-loop coefficients of the various η s.

The last discretization errors of order $\alpha_s a^2 \bar{\Lambda}^2$ stem from Eqs. (B26)–(B27). At the tree level, the numerators are 1, and in the denominators $m_3 = m_2$. At the one-loop level, mismatches appear

$$\mathbf{error}_{33} = -a^2 \frac{1}{3} (\mu_\pi^2 - \mu_G^2) f_{33}(m_{0c} a, m_{0b} a), \quad (\text{B37})$$

where f_{33} is of order α_s . Because, on the one hand, the mismatch vanishes as $a \rightarrow 0$, yet, on the other, the lattice contribution freezes out as the masses become large, we propose the following Ansatz:

$$f_{33}(m_{0c} a, m_{0b} a) = \frac{\alpha_s}{2(1 + m_{0c} a)2(1 + m_{0b} a)}. \quad (\text{B38})$$

This error is likely to be smaller than the others, because $\mu_\pi^2 - \mu_G^2$ is small; cf. Sec. B 2 c.

TABLE XII. Absolute difference of $h_{A_1}(1)$ from mismatches in the heavy-quark Lagrangian and current, estimating HQET quantities E , R_1 , R_2 with Λ^2 , $\Lambda = 450$ MeV, and taking $\mu_\pi^2 = 0.424$ GeV² and $\mu_G^2 = 0.364$ GeV². To obtain the totals, we use three uncorrelated f_B terms and two f_X . The total difference is estimated using the $a = 0.09$ fm lattice as a baseline. The right-most column shows the difference in the data between $h_{A_1}(1)$ on a given lattice and the value at $a \approx 0.09$ fm, computed at $m_x = 0.2m'_s$ as in Fig. 7.

a (fm)	$\alpha_V(q^*)$	$m_{0b}a$	$m_{0c}a$	B	X	Total	Data
0.15	0.340	3.211	0.699	0.020	0.0102	0.022	0.0072(81)
0.12	0.300	2.462	0.532	0.009	0.0044	0.010	0.0087(71)
0.09	0.261	1.664	0.362	–	–	–	–
0.06	0.220	1.123	0.240	0.003	0.0035	0.005	0.0033(82)
0.045	0.198	0.808	0.176	0.004	0.0046	0.006	0.0042(69)

c. HQET matrix elements

We have good estimates for μ_π^2 and μ_G^2 , because they appear in the heavy-quark expansions of the meson masses and of kinematic distributions of inclusive semileptonic decays. From the pseudoscalar-vector-meson mass difference

$$\mu_G^2 = \frac{3}{4}(M_{B^*}^2 - M_B^2) = 0.364 \text{ GeV}^2 = (603 \text{ MeV})^2, \quad (\text{B39})$$

which can be taken to be exact. Recent fits to inclusive $B \rightarrow X_c l \nu$ and $B \rightarrow X_s \gamma$ distributions yield a value for the kinetic energy (in the “kinetic” scheme) [91]

$$\mu_\pi^2(1 \text{ GeV}) = 0.424 \pm 0.042 \text{ GeV}^2 = (651 \pm 32 \text{ MeV})^2. \quad (\text{B40})$$

Thus, we have $\mathbf{error}_{33} \approx 0.0015$ (on lattices with $a \approx 0.09$ fm). We do not have estimates for D , E , R_1 , and R_2 as good as Eqs. (B39) and (B40), but they satisfy sum rules such that $D > 0$, $R_1 > \max(R_2, -3R_2)$.

3. Error estimation

We would now like to combine the sources of heavy-quark discretization errors into a total

$$\mathbf{error} = \bigoplus_i \mathbf{error}_i(m_0 a), \quad (\text{B41})$$

where \bigoplus denotes sum in quadrature over independent terms in \mathbf{error}_B , \mathbf{error}_X , and \mathbf{error}_{33} . With the error function f_X derived and reasonable Ansätze for f_B and f_{33} , the crucial ingredient in these estimates is the value chosen for $\bar{\Lambda}$, estimating the needed HQET matrix elements to be of order $\bar{\Lambda}^2$. Below we study our data and choose $\bar{\Lambda}$ to reproduce the observed lattice-spacing dependence. We follow the detailed derivation given above and use μ_π^2 and μ_G^2 for \mathbf{error}_X and \mathbf{error}_{33} . On the fine lattices ($a \approx 0.09$ fm), we take the typical $\alpha_V(q^*)$ to be 0.261, as in Table V, and we use one-loop running to obtain $\alpha_V(q^*)$ at the other lattice spacings.

The discretization formulas can be re-applied to estimate the difference between $\rho_{A^j} \sqrt{R_{A_1}}$ on a lattice of spacing a vs. the value on a reference lattice. Table XII shows such differences

TABLE XIII. Absolute error on $h_{A_1}(1)$ from mismatches in the heavy-quark Lagrangian and current, estimating HQET quantities E , R_1 , R_2 with Λ^2 , $\Lambda = 450$ MeV, and taking $\mu_\pi^2 = 0.424$ GeV² and $\mu_G^2 = 0.364$ GeV². To obtain the totals, we use three uncorrelated f_B terms and two f_X .

a (fm)	$\alpha_V(q^*)$	m_{0ba}	m_{0ca}	B	X	Total
0.150	0.340	3.211	0.699	0.020	0.016	0.026
0.120	0.300	2.462	0.532	0.017	0.011	0.020
0.090	0.261	1.664	0.362	0.014	0.006	0.016
0.060	0.220	1.123	0.240	0.009	0.003	0.010
0.045	0.198	0.808	0.176	0.007	0.001	0.007

with $\bar{\Lambda} = 450$ MeV and the fine ($a \approx 0.090$ fm) lattice as the reference. The variation is similar to, albeit slightly larger than, the observed lattice-spacing dependence in Fig. 7, as one can see by comparing the columns labeled “Total” and “Data” in Table XII. Guided in this way, Table XIII shows the total error with $\bar{\Lambda} = 450$ MeV. On the superfine lattice, the error is 1%, which we quote in Sec. VII as the heavy-quark discretization error on $h_{A_1}(1)$. This estimate is neither overly cautious ($\bar{\Lambda}$ is justified by the data) nor aggressive (we could have pushed $\bar{\Lambda}$ to be as small as the data would tolerate, or taken the error estimate of 0.7% from the ultrafine lattice spacing).

Appendix C: Heavy-quark Mass Tuning and Hyperfine Splitting

Our method for tuning κ for charm and bottom quarks closely follows that of Refs. [48, 51], where further details can be found. Here, however, we use a mass-independent scale-setting scheme, determining r_1/a , for each a , at the physical sea-quark masses $\hat{m} = m_s/27$ and m_s . Before we used a mass-dependent set up, taking r_1/a on each ensemble at the simulation sea masses \hat{m}' and m'_s . The new method compensates for mistunings in the sea-quark masses. We also use a new method for smoothing the lattice-spacing dependence that reduces errors, particularly at smaller lattice spacings. Finally, these second-generation tunings also have higher statistical precision than was available in Refs. [48, 51].

We start with the dispersion relation for a heavy-light meson on the lattice [47]

$$E^2(\mathbf{p}) = M_1^2 + \frac{M_1}{M_2} \mathbf{p}^2 + \frac{1}{4} A_4 (a\mathbf{p}^2)^2 + \frac{1}{3} A_4' a^2 \sum_{j=1}^3 |p_j|^4 + \dots, \quad (\text{C1})$$

where

$$M_1 \equiv E(\mathbf{0}) \quad (\text{C2})$$

is called the rest mass, and the kinetic mass is given by

$$M_2^{-1} \equiv 2 \left. \frac{\partial E(\mathbf{p})}{\partial p_j^2} \right|_{\mathbf{p}=\mathbf{0}}. \quad (\text{C3})$$

These meson masses M_1 and M_2 differ from corresponding quark masses, m_1 and m_2 , by binding-energy effects. The bare mass or, equivalently, the hopping parameter κ must be adjusted so that these masses reproduce an experimental charmed or b -flavored meson

mass. When M_1 and M_2 differ, as they do when $m_Q a \not\ll 1$, one must choose. Weak matrix elements are unaffected by the heavy-quark rest mass m_1 [53], so it does not make sense to adjust the bare mass to M_1 . On the other hand, as seen in Appendix B, the analysis of discretization effects using HQET makes M_2 the natural choice. We therefore focus on M_2 , adjusting κ to the strange pseudoscalars D_s and B_s , extrapolated to physical sea-quark masses, both because the signal degrades for lighter valence-quark masses and because this avoids introducing an unnecessary systematic uncertainty due to a chiral extrapolation in the valence-quark mass.

1. Tuning from the dispersion relation on the $\hat{m}'/m'_s = 0.2$ ensembles

We outline tuning the charm and bottom κ values with the following steps, which are described in more detail below. We work at all available lattice spacings with the $\hat{m}'/m'_s = 0.2$ ensembles.

- We have generated correlators for heavy-light pseudoscalar mesons at multiple κ values and with light-quark masses bracketing the tuned strange quark mass on the ensemble with $\hat{m}'/m'_s = 0.2$ at each of the lattice spacings $a \approx 0.045, 0.06, 0.09, 0.12$ and 0.15 fm. The charm- and bottom-quark mass regions are bracketed with at least three κ values each. In general, the available two-point data are a mix of results from κ tuning only production runs and results from full analysis production runs.
- Ground-state energies $aE(a\mathbf{p})$ for a range of $a\mathbf{p}$ were determined by (constrained) chi-square minimization fits including local-local, smeared-local and smeared-smeared (source-sink) two-point functions.
- The energies E are fit to the dispersion relation in Eq. (C1) in constrained chi-square minimizations using prior distributions for the coefficients M_1/M_2 , A_4 and $A_{4'}$ motivated by the tree-level dispersion relation for a clover heavy quark with estimated corrections for binding energy effects in a heavy-light meson [51].
- We linearly adjust each meson kinetic mass

$$M_2(m_q) = M_2(m_s) + C_v(m_q - m_s)/m_s \quad (\text{C4})$$

to get the value corresponding to the physical valence strange quark $m_q = m_s$ listed in Table XIV for each ensemble. The C_v are determined either by interpolation of the lattice results or estimated from the experimental meson masses and the physical quark masses.

- On the asqtad ensembles, the mass m'_s of the heaviest sea-quark flavor can differ significantly from the physical strange quark mass, m_s . We correct linearly for this sea-quark mass variation:

$$M_2(\hat{m}', m'_s) = M_2(\hat{m}, m_s) + C_s(2\hat{x} + x_s) \quad (\text{C5})$$

where $M_2(\hat{m}, m_s)$ is the meson mass in the limit of physical sea-quark masses, $\hat{x} = (\hat{m}' - \hat{m})/m_s$, and $x_s = (m'_s - m_s)/m_s$. The average physical mass is $\hat{m} = (m_u + m_d)/2$ while \hat{m}' is the sea-quark mass used in simulations. We estimate $r_1 C_s \approx 0.02$ for the D_s and $r_1 C_s \approx 0.012$ for the B_s based upon an analysis of the sea-quark mass dependence on the $a \approx 0.12$ fm lattice, and we take the physical mass \hat{m} from Table XIV.

TABLE XIV. Ensembles with sea-quark $\hat{m}'/m'_s = 0.2$ that are used in κ tuning, smoothed values of r_1/a and the physical quark masses, m_s and $\hat{m} = (m_u + m_d)/2$ obtained from the analysis of the light spectrum and decay constants [66].

$\approx a$ (fm)	r_1/a	β	am'_s	$a\hat{m}'$	am_s	$a\hat{m}$
0.15	2.221530	6.572	0.0484	0.0097	0.04185	0.001508
0.12	2.738591	6.76	0.05	0.01	0.03357	0.001215
0.09	3.788732	7.09	0.031	0.0062	0.02446	0.0008922
0.06	5.353063	7.47	0.018	0.0036	0.01751	0.0006401
0.045	7.208234	7.81	0.014	0.0028	0.01298	0.0004742

- On each ensemble, the lattice masses $M_2(\kappa_h, m_s)$, adjusted to the correct (valence and sea) strange quark mass, must be fit to an interpolating function prior to implicitly solving for the κ value needed to match the lattice M_2 to the experimental value of the D_s or B_s meson mass. We have tested two different interpolating functions, finding negligible difference in the resulting tuned κ values. For the first fit-function we use the same HQET-inspired form as in our previous tuning analyses:

$$M_2(\kappa) = \Lambda + m_2(\kappa) + \frac{\lambda_1}{m_2(\kappa)} \quad (\text{C6})$$

where quark mass m_2 is computed to tree level. The parameters Λ and λ_1 are determined in a chi-square minimization. The set of two parameters are determined separately for charm and bottom. The second fit function is quadratic or linear in the tree-level bare quark mass am_0 . Again, the coefficients of the best fit are determined separately for charm and bottom. In Fig. 8 we show examples of polynomial interpolations of $r_1 M_2(\kappa)$ and indicate values corresponding to the known D_s and B_s masses.

- We use MILC's smoothed r_1/a measurements and the value $r_1 = 0.3117(22)$ fm [51] to set the lattice spacing in our determinations of κ_c and κ_b .

The process outlined above is used in two separate analyses. Analysis A is based on the two-point functions listed in Table XV and a block-elimination jackknife with block sizes ranging from 5 to 32 to estimate statistical errors. Analysis B uses the two-point functions listed in Table XVI together with a bootstrap procedure in the error analysis. For several ensembles, Analysis B adds two additional (a charm-like and a bottom-like) κ values from the two-points generated in our full analysis campaign. The rest and kinetic masses from the two different analyses for the five $\hat{m}'/m'_s = 0.2$ ensembles with different lattice spacing are listed in Tables XVII-XXI. The charm and bottom κ values obtained in the two analyses are tabulated, with statistical errors, in Table XXII. The table also shows a comparison of κ values obtained from the HQET-inspired interpolation versus an interpolation quadratic in m_0 . The tabulated (quadratic) results are plotted in Figure 9 for comparison. The results from the two analyses are statistically consistent (with highly correlated statistical errors). We take a weighted average from the two analyses (see Table XXII) and use the resulting charm and bottom κ values in subsequent steps of the analysis.

TABLE XV. Analysis A of $\hat{m}'/m'_s = 0.2$ ensembles, configurations \times sources and two-point valence masses and κ values. In all cases we use local-local, smeared-local, and smeared-smeared (source-sink) two-point functions in fits. The number of states (+ opposite parity states) and time range fit are shown. Where three fit ranges are shown, the first refers to the smeared-smeared correlator, the second, the smeared-local correlator, and the third, the local-local correlator. Where only one range is shown, all three correlators are fit to the same range. Two-point functions with momenta $|\mathbf{p}| \leq |2|2\pi/L$ are included in the analysis.

a (fm)	cfgs \times sracs	am_q	κ	states t range
0.15	631 \times 8	0.0387, 0.0484	0.070, 0.076, 0.080	2 + 2 [5, 17]
		0.0387, 0.0484	0.090, 0.100, 0.115	2 + 2 [6, 18]
		0.0387, 0.0484	0.115, 0.122, 0.125	2 + 2 [8, 20]
0.12	2259 \times 4	0.340, 0.370	0.074, 0.086, 0.098	2 + 2 [9, 16]
		0.340, 0.370	0.1175, 0.1200, 0.1225	2 + 2 [11, 21]
0.09	1912 \times 8	0.0250, 0.0270	0.090, 0.092, 0.094	2 + 2 [10, 20]
		0.0250, 0.0270	0.1240, 0.1255, 0.1270	3 + 3 [12, 24]
		0.0261, 0.0310	0.1276, 0.979	3 + 3 [12, 20]
0.06	670 \times 4	0.0188	0.100, 0.106, 0.122	2 + 2 [15, 31]
		0.0188	0.124, 0.127, 0.130	2 + 2 [20, 30]; [24, 34]; [28, 38]
0.045	801 \times 4	0.130, 0.135	0.106, 0.111, 0.116	2 + 2 [18, 36]
		0.130, 0.135	0.128	2 + 2 [19, 35]; [20, 36]; [20, 36]
		0.130, 0.135	0.130, 0.132	2 + 2 [20, 36]

2. Smoothing and extending κ tuning to other ensembles

In the second step of our κ tuning analysis we improve the raw tuned results by smoothing them as a function of lattice spacing and by adding the constraint that the *rest* masses M_1 extrapolate to their physical values at zero lattice spacing. This treatment gives the small adjustments in the central values and the reduction in error, shown in the last column of Table XXII. The improvement in error gets progressively better as the lattice spacing is decreased.

The continuum extrapolation of the rest masses M_1 adds a useful constraint to the κ tuning analysis, since the rest masses are determined to much higher statistical accuracy than the kinetic masses M_2 . On each ensemble with fixed lattice spacing a/r_1 , their dependence on heavy valence quark κ can be described accurately with an interpolating function $M_1(\kappa, a/r_1)$, which we take to be quadratic in the bare heavy-quark mass and which we determine separately for charm-like and bottom-like masses. Thus, on each ensemble, a tuned value of κ and its error implies, through interpolation, an inferred value of $M_1(a/r_1)$ with appropriately propagated error. (The errors from the interpolation were negligible compared with the errors arising from uncertainties in the tuned values of κ themselves.) The inferred rest masses are shown in Table XXIII for the D_s and B_s on the ensembles with $\hat{m}'/m'_s = 0.2$, and are uncorrected for unphysical sea-quark masses. We determine the sea-quark mass correction following Eq. (C5), but with a coefficient C'_s appropriate for the rest mass. The resulting sea-quark-mass correction is shown in Table XXIII. Our smoothing

TABLE XVI. Analysis B of $\hat{m}'/m'_s = 0.2$ ensembles, configurations \times sources and two-point valence masses and κ values. In all cases we use local-local, smeared-local, and smeared-smeared (source-sink) 2-pt functions in fits. The number of states (+ opposite parity states) and time range fit are shown. Two-point functions with momenta $|\mathbf{p}| \leq |3|2\pi/L$ are fit.

a (fm)	cfgs \times srcs	am_q	κ	states	t range
0.15	631 \times 8	0.0484	0.070, 0.076, 0.080	3 + 3	[6, 22]
		0.0484	0.085, 0.090, 0.094, 0.110	3 + 3	[6, 22]
		0.0484	0.115, 0.122, 0.125	3 + 3	[6, 22]
	631 \times 24	0.0484	0.0781, 0.1218	3 + 3	[6, 22]
0.12	2259 \times 4	0.349	0.0820, 0.0860, 0.0901	3 + 3	[6, 24]
		0.349	0.1230, 0.1254, 0.1280	3 + 3	[6, 28]
0.09	1912 \times 8	0.0270	0.090, 0.092, 0.094	3 + 3	[12, 36]
	1931 \times 4	0.0261	0.0979	3 + 3	[12, 36]
	1912 \times 8	0.0270	0.1240, 0.1255, 0.1270	3 + 3	[12, 40]
	1931 \times 4	0.0261	0.1276	3 + 3	[12, 40]
0.06	670 \times 4	0.0188	0.100, 0.106, 0.122	3 + 3	[26, 48]
	673 \times 8	0.0188	0.1052	3 + 3	[26, 48]
	670 \times 4	0.0188	0.124, 0.127, 0.130	3 + 3	[22, 52]
	673 \times 8	0.0188	0.1296	3 + 3	[22, 52]
0.045	801 \times 4	0.130	0.106, 0.111, 0.1143, 0.116	3 + 3	[19, 60]
		0.130	0.128, 0.130, 0.1310, 0.132	3 + 3	[19, 70]

procedure then fits the inferred, adjusted values of $M_1(a/r_1)$ to a smooth function of lattice spacing a/r_1 , with the constraint that the intercept $M_1(0)$ agrees with the physical mass.

For the B_s we use the empirically chosen form

$$M_1(a^2; B_s) = M(B_s)_{\text{phys}} + b_1 x + b_2 x^2 \quad (\text{C7})$$

where $x = (a/r_1)^2/[0.1 + (a/r_1)^2]$. In units of the physical B_s meson mass M this parameter becomes $x = (aM)^2/[7.3 + (aM)^2]$, which reduces the model to a quadratic in a^2 for $aM \ll 3$. The resulting fit is shown in the left panel of Fig. 10 ($\chi^2/\text{d.o.f.} = 0.4/3$, $p = 0.94$).

For charm-like masses, evidently, the value of $aM(D_s)$ is sufficiently small that a simple quadratic in $(a/r_1)^2$ suffices:

$$M_1(a^2; D_s) = M(D_s)_{\text{phys}} + c_1 \frac{a^2}{r_1^2} + c_2 \frac{a^4}{r_1^4} \quad (\text{C8})$$

The resulting fits are shown in the right panel of Fig. 10 ($\chi^2/\text{d.o.f.} = 2.4/3$, $p = 0.49$).

We then use the best fits to determine the smoothed values of M_1 at each lattice spacing. Ensemble by ensemble, through the valence quark mass interpolation, these smoothed values, in turn, provide the smoothed κ s for each $0.2m'_s$ ensemble. They are recorded in Table XXII.

Finally, we need to extend our determination of κ_c and κ_b to predict their values for ensembles with values of \hat{m}'/m'_s other than 0.2. Because we are using a mass-independent

TABLE XVII. Results for rest and kinetic masses (in lattice units) on the $a \approx 0.15$ fm ensemble.

κ	Analysis A			Analysis B		
	am_q	aM_1	aM_2	am_q	aM_1	aM_2
0.125	0.04213	1.1459(7)	1.284(14)	0.0484	1.1566(6)	1.295(15)
0.122		1.2324(9)	1.406(24)		1.2427(7)	1.419(18)
0.115		1.4182(10)	1.717(22)		1.4282(9)	1.719(28)
0.110		–	–		1.5515(10)	1.938(37)
0.100		1.7759(14)	2.524(56)		–	–
0.090		1.9991(19)	3.165(101)		2.0077(18)	3.003(100)
0.085		–	–		2.1181(21)	3.290(123)
0.080		2.2193(22)	3.764(131)		2.2287(23)	3.629(156)
0.076		2.3087(24)	4.077(155)		2.3182(26)	3.901(182)
0.070		2.4444(29)	4.654(232)		–	–

TABLE XVIII. Results for rest and kinetic masses (in lattice units) on the $a \approx 0.12$ fm ensemble.

κ	Analysis A			Analysis B		
	am_q	aM_1	aM_2	am_q	aM_1	aM_2
0.1280	0.03357		–	0.0349	0.9239(3)	1.008(8)
0.1254			–		1.0066(3)	1.120(10)
0.1230			–		1.0787(4)	1.223(13)
0.1225		1.0918(4)	1.228(15)		–	–
0.1200		1.1628(4)	1.327(17)		–	–
0.1175		1.2309(5)	1.429(23)		–	–
0.0980		1.7040(9)	2.378(69)		–	–
0.0901		–	–		1.8837(11)	3.000(123)
0.0860		1.9728(16)	3.064(137)		1.9760(11)	3.181(152)
0.0820		–	–		2.0651(12)	3.404(197)
0.0740		2.2419(24)	4.037(261)		–	–

scheme, we interpolate only in β , where we note that the variation of β with sea quark mass (at approximately constant lattice spacing) is very slight. Because κ_c and κ_b are tuned to masses adjusted to the physical sea-quark masses, this mass-independent scheme is based on physical hadron (π , K , D_s , and B_s) masses and physical f_π at all lattice spacings. To predict the κ values at other β 's the functions $\kappa_c(\beta)$ and $\kappa_b(\beta)$ are fit to a cubic spline. The spline is used *only* to determine the derivatives $d\kappa_c/d\beta$ and $d\kappa_b/d\beta$ at the β_i 's for the five $0.2m'_s$ ensembles. The derivatives are, in turn, used to obtain κ_c and κ_b at the slightly shifted β values for each of the four lattice spacings where we need them. The results are the final smoothed κ values listed in Table XXIV.

TABLE XIX. Results for rest and kinetic masses (in lattice units) on the $a \approx 0.09$ fm ensemble.

κ	Analysis A			Analysis B		
	am_q	aM_1	aM_2	am_q	aM_1	aM_2
0.1276	0.02468	0.7698(3)	0.798(6)	0.0261	0.7720(2)	0.810(7)
0.1270		0.7900(3)	0.842(9)	0.0270	0.7940(2)	0.844(5)
0.1255		0.8392(3)	0.895(8)		0.8428(2)	0.907(7)
0.1240		0.8862(4)	0.953(10)		0.8898(2)	0.971(8)
0.0979		1.5306(12)	2.210(83)	0.0261	1.5577(7)	1.975(45)
0.0940		1.6450(10)	2.390(70)	0.0270	1.6479(7)	2.306(67)
0.0920		1.6902(10)	2.498(84)		1.6931(7)	2.411(79)
0.0900		1.7353(10)	2.605(95)		1.7382(7)	2.525(88)

TABLE XX. Results for rest and kinetic masses (in lattice units) on the $a \approx 0.06$ fm ensemble.

κ	Analysis A			Analysis B		
	am_q	aM_1	aM_2	am_q	aM_1	aM_2
0.130	0.01777	0.5518(4)	0.563(5)	0.0188	0.5536(3)	0.570(4)
0.1296		–	–		0.5693(2)	0.582(4)
0.127		0.6593(5)	0.678(11)		0.6608(4)	0.696(7)
0.124		0.7568(7)	0.790(16)		0.7581(5)	0.817(10)
0.122		–	–		–	–
0.112		1.0924(13)	1.325(56)		1.0935(12)	1.271(33)
0.106		1.2412(18)	1.621(95)		1.2430(14)	1.536(52)
0.1052		–	–		1.2640(9)	1.543(49)
0.100		1.3833(23)	1.975(164)		1.3856(18)	1.845(75)

TABLE XXI. Results for rest and kinetic masses (in lattice units) on the $a \approx 0.045$ fm ensemble.

κ	Analysis A			Analysis B		
	am_q	aM_1	aM_2	am_q	aM_1	aM_2
0.132	0.01298	0.3818(2)	0.394(3)	0.0130	0.3819(2)	0.384(1)
0.1310		–	–		0.4239(2)	0.429(2)
0.130		0.4631(3)	0.484(5)		0.4632(2)	0.470(2)
0.128		0.5368(4)	0.564(7)		0.5370(3)	0.550(3)
0.116		0.9025(6)	1.056(32)		0.9021(6)	1.021(16)
0.1143		–	–		0.9480(5)	1.056(18)
0.111		1.0336(6)	1.266(48)		1.0331(8)	1.225(26)
0.106		1.1576(7)	1.535(75)		1.1573(9)	1.446(37)

3. Scale error

As noted above, we take $r_1 = 0.3117(22)$ fm [51]. The error in the scale determination introduces an error in converting the experimental mass to aM_2 , which propagates, in turn, to the tuned κ s. The systematic error on the tuned κ s due to the uncertainty in the lattice scale determination is therefore obtained by changing r_1 from its central value by one standard deviation and propagating this change through our κ tuning analysis. Our final tuned κ_b and κ_c results including both statistical and r_1 systematic errors are shown in Table XXIV. We note that the derivative of the κ s with respect to r_1 is negative. So increasing r_1 by 0.0022 causes κ to decrease by the amount shown. This exercise was done only on the $0.2m'_s$ ensembles. We assume that the errors are the same for ensembles at nearby β (nearly same lattice spacing).

The correct way to propagate the scale error to the dimensionful quantities that we calculate is first to compute the physical quantity for a fixed r_1 , propagating only the statistical error in κ (*i.e.*, not first combining statistical and scale errors in some way),

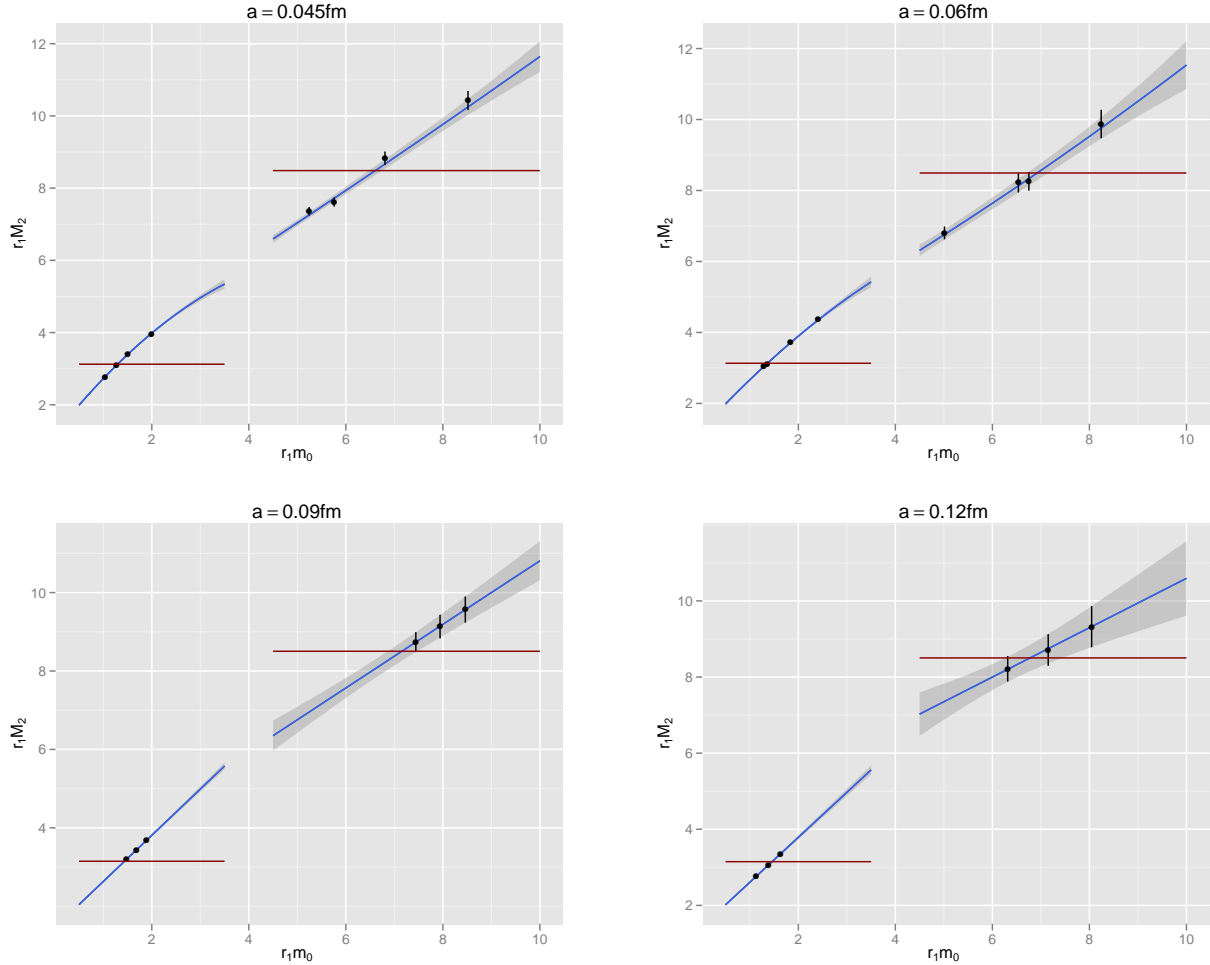


FIG. 8. Interpolation of $r_1 M_2(\kappa)$ to the corresponding physical D_s and B_s meson masses (indicated by the horizontal lines). Separate (quadratic or linear) interpolations are performed for charm and bottom. These results are from Analysis B. The figure for the $a \approx 0.15$ fm lattice is not shown.

TABLE XXII. Charm (κ_c) and bottom (κ_b) results from an analysis of the energy-momentum dispersion relation on the $\hat{m}'/m'_s = 0.2$ ensembles. Results from analyses A and B are listed with statistical errors. Under analysis A we tabulate κ values found using an HQET-inspired interpolating function. The weighted average of A:poly and B:poly results and the results after the smoothing fit are listed. The third column shows κ values used in the production campaign.

a (fm)	system	production	A:HQET	A:poly	B:poly	wt. avg.	smoothed
0.15	charm	0.1218	0.12210(30)	0.12187(33)	0.12247(22)	0.12229(26)	0.12237(26)
0.12		0.1254	0.12452(47)	0.12464(57)	0.12467(25)	0.12467(32)	0.12423(15)
0.09		0.1276	0.12721(14)	0.12708(13)	0.12731(13)	0.12720(13)	0.12722(9)
0.06		0.1296	0.12959(12)	0.12944(13)	0.12957(07)	0.12954(09)	0.12960(4)
0.045		0.1310	0.13124(10)	0.13107(10)	0.13089(03)	0.13090(04)	0.130921(16)
0.15	bottom	0.0781	0.0803(11)	0.0792(18)	0.0762(19)	0.0778(18)	0.0775(16)
0.12		0.0901	0.0864(12)	0.0856(18)	0.0878(29)	0.0862(22)	0.0868(9)
0.09		0.0979	0.0971(8)	0.0971(09)	0.0952(13)	0.0965(10)	0.0967(7)
0.06		0.1052	0.1064(15)	0.1067(14)	0.1046(08)	0.1051(10)	0.1052(5)
0.045		0.1143	0.1125(10)	0.1129(10)	0.1116(04)	0.1118(05)	0.1116(3)

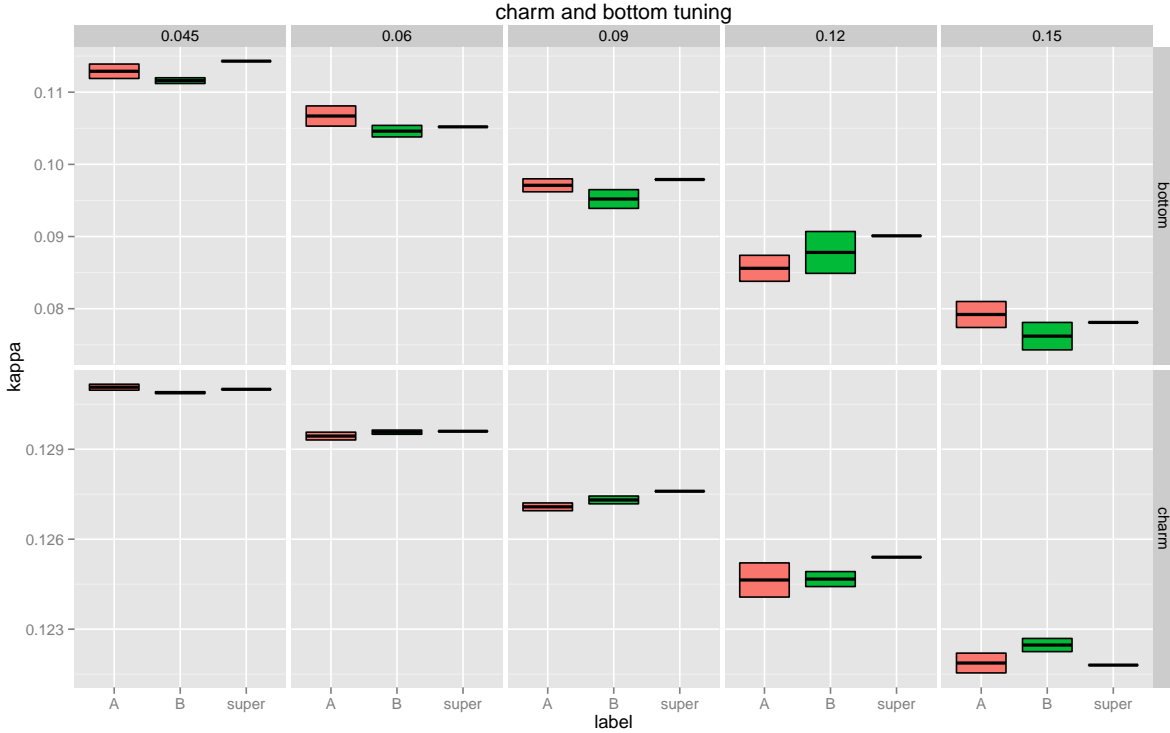


FIG. 9. Comparison of charm and bottom κ values from analyses A (red) and B (green) together with the κ values used in the production campaign.

TABLE XXIII. Rest masses of D_s and B_s interpolated to the respective weighted average κ_c and κ_b values for each of the $\hat{m}'/m'_s = 0.2$ ensembles in the tuning sample. σ_{tune} is the error propagated from the uncertainty in the weighted averages of κ_c and κ_b and δM_{sea} is the correction applied to the rest-masses due to the extrapolation to the physical sea-quark masses. The rest-masses listed in columns 2 and 5 are the results obtained before applying the sea-quark mass correction. Masses are in MeV.

a/r_1	$M_1(D_s)$	σ_{tune}	δM_{sea}	$M_1(B_s)$	σ_{tune}	δM_{sea}
0.4501	1721.2	10.4	-11.0	3190.0	57.2	-6.7
0.3652	1779.9	16.9	-20.7	3411.9	87.0	-12.6
0.2639	1878.7	10.5	-14.1	3801.2	58.5	-8.6
0.1868	1927.5	11.3	-7.3	4280.3	82.8	-4.4
0.1387	1950.2	7.4	-9.0	4622.1	59.1	-5.5

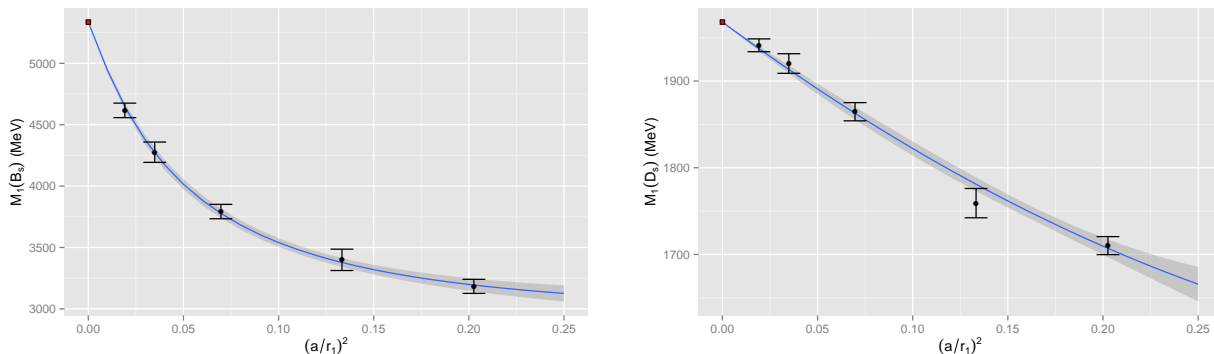


FIG. 10. Lattice rest masses (in MeV) for the B_s (left) and D_s (right) at physical valence and sea-quark masses as a function of $(a/r_1)^2$.

and then to recompute the same quantity with the shifted κ and shifted r_1 . The difference in the central values of the final result is, then, the r_1 systematic error.

4. $D_s^*-D_s$ and $B_s^*-B_s$ hyperfine splittings

The hyperfine splittings, $M(D_s^*) - M(D_s)$ and $M(B_s^*) - M(B_s)$, are sensitive to the heavy-quark mass and to discretization effects, and they therefore provide a good test of both our analysis of discretization errors and of our κ -tuning analysis. As with the pseudoscalar mesons D_s and B_s , we made sea-quark mass adjustments for the vector mesons D_s^* and B_s^* , as discussed above. We computed the hyperfine splitting at the physical strange quark mass over a range of valence κ values. For purposes of interpolation we fit the rest-mass splitting on each ensemble as a quadratic in $1/(am_0)$, the inverse bare quark mass. This fitting function works well over the entire range of valence κ s from charm to bottom. After interpolation we apply a correction for heavy-quark discretization errors to leading order in heavy-quark effective theory as described in [48]. The resulting values are listed in Tables XXV and XXVI and are shown in Fig. 11. An error budget is also tabulated. For the remaining heavy-quark discretization error (beyond leading order), we used the full leading-order correction at

TABLE XXIV. Final, smoothed mass-independent κ_c and κ_b values and production values for various ensembles. The second error reflects the uncertainty in the r_1 determination. See Sec. C 3 for the preferred way to handle it. Smoothing is discussed in Sec. C 2.

$\approx a$ (fm)	Ensemble		Tuned (final)		Production	
	β	\hat{m}'/m'_s	κ_c	κ_b	κ_c	κ_b
0.15	6.566	0.1	0.12231(26)(20)	0.0772(16)(3)	–	–
	6.572	0.2	0.12237(26)(20)	0.0775(16)(3)	0.1218	0.0781
	6.586	0.4	0.12252(26)(20)	0.0780(16)(3)	–	–
0.12	6.76	0.1	0.12423(15)(16)	0.0868(9)(3)	0.1254	0.0901
	6.76	0.14	0.12423(15)(16)	0.0868(9)(3)	0.1254	0.0901
	6.76	0.2	0.12423(15)(16)	0.0868(9)(3)	0.1254	0.0901
	6.79	0.4	0.12452(15)(16)	0.0879(9)(3)	0.1259	0.0918
0.09	7.075	0.05	0.12710(9)(14)	0.0964(7)(3)	0.1275	0.0976
	7.08	0.1	0.12714(9)(14)	0.0965(7)(3)	0.1275	0.0976
	7.085	0.14	0.12718(9)(14)	0.0966(7)(3)	0.1275	0.0977
	7.09	0.2	0.12722(9)(14)	0.0967(7)(3)	0.1276	0.0979
	7.10	0.3	0.12730(9)(14)	0.0970(7)(3)	–	–
	7.11	0.4	0.12737(9)(14)	0.0972(7)(3)	0.1277	0.0982
0.06	7.46	0.1	0.12955(4)(11)	0.1050(5)(2)	0.1296	0.1052
	7.465	0.14	0.12957(4)(11)	0.1051(5)(2)	0.1296	0.1052
	7.47	0.2	0.12960(4)(11)	0.1052(5)(2)	0.1296	0.1052
	7.475	0.3	0.12962(4)(11)	0.1052(5)(2)	–	–
	7.48	0.4	0.12964(4)(11)	0.1054(5)(2)	0.1295	0.1048
0.045	7.81	0.2	0.130921(16)(70)	0.1116(3)(2)	0.1310	0.1143

0.06 fm. Error contributions are combined in quadrature. Our results for the splittings are extrapolated three ways to zero lattice spacing: The values corrected for heavy-quark discretization errors are extrapolated linearly in $(a/r_1)^2$. The uncorrected values are similarly extrapolated. The corrected values are simply averaged (extrapolated with slope fixed to zero). All results are consistent. They are compared with the experimental values given in the last line of each table [1]. The largest uncertainty comes from the adjustment from the simulation sea-quark masses to the physical sea-quark masses. For the D_s hyperfine splitting, the prediction is well within 1σ of the experimental value, and for the B_s , about 1.3σ below (lower panels of Fig. 11). Without the leading heavy-quark correction, the extrapolated result for the D_s splitting is also well within 1σ of the experimental value and for the B_s , slightly more than 1.3σ below (upper panels), but the extrapolation model (linear in $(a/r_1)^2$) is then less reliable.

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TABLE XXV. Hyperfine splitting $\Delta M_{\text{hfs}}(D_s) = M_{D_s^*} - M_{D_s}$ in MeV at the physical valence- and sea-quark masses as a function of a/r_1 . The splittings shown in the second column include a correction for heavy-quark discretization errors to leading order [48], while the third column shows the uncorrected value. The remaining columns give the error budget. Shown are the fit error, charm mass tuning error, sea-quark mass adjustment, the combination (in quadrature) of these three sources of statistical error, the systematic scale error, the systematic heavy-quark discretization error, and the combination (in quadrature) of the statistical and systematic errors. The three rows at zero lattice spacing give, respectively, the value obtained by linear extrapolation of the corrected splittings in $(a/r_1)^2$, by similarly extrapolating the uncorrected splittings, and by taking the mean of the corrected splittings, and the last row gives the experimental value.

a/r_1	$\Delta M_{\text{hfs}}(D_s)$	uncorrected	fit	tune	sea	quark	net stat.	r_1	scale	hvy. qk.	total
0.4501	145.4	136.1	1.4	1.0	4.1	4.5	2.1	1.8	5.2		
0.3652	142.8	136.3	6.6	0.9	7.7	10.1	1.8	1.8	10.5		
0.2639	144.9	141.0	1.9	0.7	5.2	5.6	1.9	1.8	6.2		
0.1868	143.9	141.7	3.4	3.7	2.8	5.8	2.0	1.8	6.4		
0.1387	148.1	146.7	2.3	2.3	3.4	4.7	2.1	1.8	5.4		
0.0000	146(4)	corrected									
0.0000	145(4)	uncorrected									
0.0000	146(3)	mean									
expt	143.8(4)										

TABLE XXVI. The same as Table XXV, but for the hyperfine splitting $\Delta M_{\text{hfs}}(B_s) = M_{B_s^*} - M_{B_s}$.

a/r_1	$\Delta M_{\text{hfs}}(B_s)$	uncorrected	fit	tune	sea	quark	net stat.	r_1	scale	hvy. qk.	total
0.4501	43.6	39.2	1.4	1.3	3.5	4.0	0.6	1.4	4.3		
0.3652	44.0	40.6	2.8	0.9	6.8	7.4	0.6	1.4	7.5		
0.2639	45.7	43.3	1.2	0.7	4.7	4.9	0.7	1.4	5.1		
0.1868	40.5	39.1	2.8	0.7	2.5	3.8	0.6	1.4	4.1		
0.1387	45.8	44.7	2.4	0.5	3.0	3.9	0.6	1.4	4.1		
0.0000	44(3)	corrected									
0.0000	43(3)	uncorrected									
0.0000	44(2)	mean									
expt	$48.7^{+2.3}_{-2.1}$										

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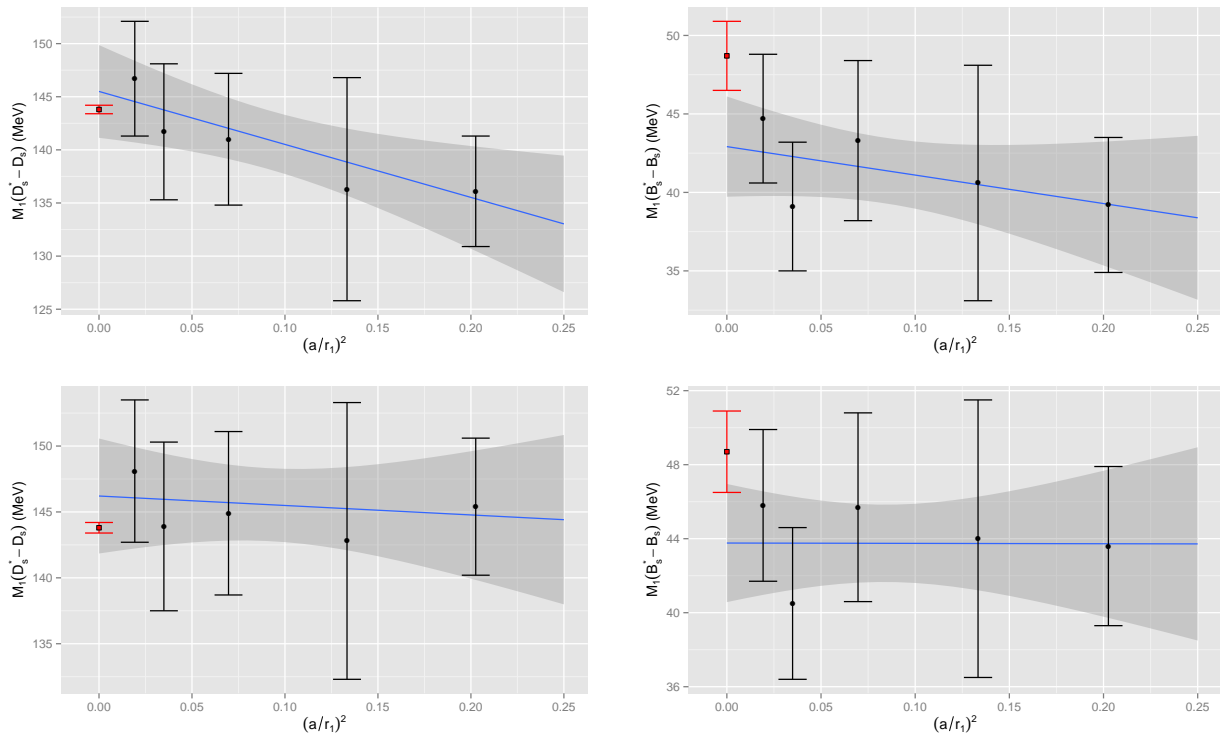


FIG. 11. Hyperfine splittings for the D_s (left) and B_s (right) systems in MeV, shown with full errors, extrapolated (linearly in $(a/r_1)^2$) to zero lattice spacing. Experimental values are indicated by the (red) points at $a = 0$. Upper panels: before correction for leading heavy-quark discretization error. Lower panels: after correction.

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