

Lattice QCD Matrix Elements for the $B_s^0 - \bar{B}_s^0$ Width Difference beyond Leading Order

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(Received 3 October 2019; accepted 22 January 2020; published 26 February 2020)

Predicting the $B_s^0 - \bar{B}_s^0$ width difference $\Delta\Gamma_s$ relies on the heavy quark expansion and on hadronic matrix elements of $\Delta B = 2$ operators. We present the first lattice QCD results for matrix elements of the dimension-7 operators $R_{2,3}$ and linear combinations $\tilde{R}_{2,3}$ using nonrelativistic QCD for the bottom quark and a highly improved staggered quark (HISQ) action for the strange quark. Computations use MILC Collaboration ensembles of gauge field configurations with $2 + 1 + 1$ flavors of sea quarks with the HISQ discretization, including lattices with physically light up or down quark masses. We discuss features unique to calculating matrix elements of these operators and analyze uncertainties from series truncation, discretization, and quark mass dependence. Finally we report the first standard model determination of $\Delta\Gamma_s$ using lattice QCD results for all hadronic matrix elements through $\mathcal{O}(1/m_b)$. The main result of our calculations yields the $1/m_b$ contribution $\Delta\Gamma_{1/m_b} = -0.022(10) \text{ ps}^{-1}$. Adding this to the leading order contribution, the standard model prediction is $\Delta\Gamma_s = 0.092(14) \text{ ps}^{-1}$.

DOI: [10.1103/PhysRevLett.124.082001](https://doi.org/10.1103/PhysRevLett.124.082001)

Oscillations of neutral mesons into their antiparticles have been important phenomena in the study of quark flavor. This flavor-changing, neutral mixing is absent in the standard model (SM) at the classical level; appearing at one-loop level it is suppressed by two powers of Fermi's constant G_F relative to hadronic and quark mass scales. A few observables are, to a high level of precision, sensitive only to short-distance physics. Within the standard model, predictions for these are reliably calculable because the dominant contribution comes from top-quark loops; there is no significant contribution from intermediate-state hadronic physics. Prime examples are in the mixing of strange mesons $K^0 - \bar{K}^0$, the indirect CP -violating ratio ϵ_K and, in beauty mesons $B_{d,s}^0 - \bar{B}_{d,s}^0$, the mass differences (equivalently, the oscillation frequencies) $\Delta M_{d,s}$. Precise experimental measurements of these, together with accurate

standard model predictions, constitute stringent tests of the SM description of quark flavor.

Beyond these observables are others, where contributions from hadronic intermediate states must be included. For example, mixing in neutral charm mesons $D^0 - \bar{D}^0$ has significant long-distance contributions due to differing flavor structure from K^0 and B^0 mixing. Predictions for heavy meson and baryon lifetimes also require theoretical treatment of long-distance effects.

The $B_s^0 - \bar{B}_s^0$ width difference $\Delta\Gamma_s$ is another example and is the focus of this Letter. Unlike the mass difference, which comes from the real part of the mixing amplitude, the width difference comes from the imaginary part which, by the optical theorem, describes the decays to real final states, primarily $b \rightarrow c\bar{c}s$ decays. Consequently, $\Delta\Gamma_s$ is dominantly due to processes with intrinsic charm and we expect it to be insensitive to new physics. Comparison between theory and experiment is a test of the theoretical methods involved, including the assumption of quark-hadron duality. Agreement here is a necessary condition for trusting these methods to reliably yield a SM prediction for quantities where new physics could contribute more prominently, e.g., in $D^0 - \bar{D}^0$ mixing.

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Predicting the SM width difference $\Delta\Gamma_s$ requires the determination of matrix elements of a nonlocal product of effective operators $H_{\text{eff}}^{\Delta F=1}$, with charm and up quarks in the virtual loops. Direct calculation of $\langle \bar{B}_s^0 | \mathcal{T} \{ H_{\text{eff}}^{\Delta F=1}(x) H_{\text{eff}}^{\Delta F=1}(0) \} | \bar{B}_s^0 \rangle$ using lattice QCD is not presently feasible. Therefore, an additional theoretical approximation is necessary in order to obtain a standard model prediction for $\Delta\Gamma_s$, namely, the heavy quark expansion (HQE). This expansion makes use of the large b -quark mass compared to the c quark and other scales in the problem such as Λ_{QCD} , and approximates the imaginary part of the matrix elements above by a power series in $1/m_b$, composed of matrix elements of local, $\Delta F = 2$ operators such as those appearing in $H_{\text{eff}}^{\Delta F=2}$ [1]. (See Ref. [2] for a recent review of the HQE applied to $\Delta\Gamma_s$.)

Matrix elements of the leading, dimension-6 operators in $H_{\text{eff}}^{\Delta F=2}$ have been calculated using lattice QCD with increasing precision, motivated by their impact on predictions for $\Delta M_{d,s}$. Results are now available from several groups [3–6] (see Ref. [7] for a review and Refs. [8,9] for sum rule calculations). The precision of these determinations has become good enough that matrix elements of higher-dimension operators are needed in order to reduce the SM uncertainty in $\Delta\Gamma_s$. Current estimates for the higher-dimension matrix elements come from the vacuum saturation approximation [2], although sum rules have also been applied [10]. The lack of any full QCD calculation of dimension-7 operators is the leading uncertainty in the standard model determination of $\Delta\Gamma_s$ [2,11].

In this Letter, we provide results of the first complete lattice QCD calculation needed for $\Delta\Gamma_s$ through $\mathcal{O}(1/m_b)$. The goal here is to replace order-of-magnitude estimates based on the vacuum saturation approximation with first principles calculations including a quantitative analysis of errors. In this first step, we neglect $\mathcal{O}(\alpha_s)$ corrections to the dimension-7 operators. Including these corrections involves a technically challenging perturbative calculation which is left as a future project.

The convention we use for the dimension-6 operators O_{1-5} is as in Ref. [6]. At higher order in the HQE, one needs matrix elements of the following operators:

$$\begin{aligned} R_0 &= O_2 + \alpha_1 O_3 + \frac{1}{2} \alpha_2 O_1, & R_1 &= \frac{m_s}{m_b} O_4 \\ R_2 &= \frac{1}{m_b^2} [\bar{b}^\alpha \bar{D}_\rho \gamma^\mu (1 - \gamma^5) D^\rho s^\alpha] [\bar{b}^\beta \gamma_\mu (1 - \gamma^5) s^\beta] \\ R_3 &= \frac{1}{m_b^2} [\bar{b}^\alpha \bar{D}_\rho (1 - \gamma^5) D^\rho s^\alpha] [\bar{b}^\beta (1 - \gamma^5) s^\beta], \end{aligned} \quad (1)$$

as well as the color-rearranged partners \tilde{R}_1 , \tilde{R}_2 , and \tilde{R}_3 . The perturbative coefficients α_1 and α_2 are given in Refs. [12–14]. Using Fierz identities and neglecting terms at higher order in $1/m_b$ we have

$$\tilde{R}_2 = -R_2 \quad \text{and} \quad \tilde{R}_3 = R_3 + \frac{1}{2} R_2. \quad (2)$$

In nonrelativistic lattice QCD, matrix elements of both sides of Eq. (2) hold exactly.

We carry out our calculations using gauge field configurations generated by the MILC Collaboration [15–17]. These include the effects of $2 + 1 + 1$ flavors of sea quarks using the highly improved staggered quark (HISQ) fermion action [18,19]. We use five separate ensembles, those labeled sets 1, 3, 4, 6, and 7 in Ref. [6] (see also Supplemental Material [20]). Two of the ensembles have all of the quark masses tuned to be close to their physical values, e.g., $m_s/m_l \approx 27$; these have lattice spacings of 0.12 and 0.15 fm. The other three ensembles span three lattice spacings from 0.09 to 0.15 fm, with unphysically large light-quark masses corresponding to pion masses of about 300 MeV, $m_s/m_l \approx 5$. Our use of three lattice spacings allows us to estimate discretization errors, and the computations done with unphysical light quark masses gives us information with which to correct any slight quark mass mistunings.

The lattice actions used are the same as in our recent study of the dimension-6 operator matrix elements [6]. Correlation functions are computed using the HISQ action for the strange quark; the valence quark mass is tuned to be closer to the physical strange mass than the value which was used for the sea strange quark. The nonrelativistic QCD (NRQCD) action [21,22] is used for the bottom quark. The action coefficients and valence quark parameters are the same as in recent work [6,22,23]. Because the determination of $\langle R_2 \rangle$ and $\langle R_3 \rangle$ here will have an $\mathcal{O}(\alpha_s)$ uncertainty due to tree-level matching between lattice and continuum regularization schemes, we only need a fraction of the statistics used in Ref. [6]. We will occasionally refer to Ref. [6] as the high-statistics companion to this work. Throughout this Letter we will use the abbreviated notation $\langle \cdot \rangle \equiv \langle B_s | \cdot | \bar{B}_s \rangle$.

Let us examine a unique feature of computing $\langle R_2 \rangle$ and $\langle R_3 \rangle$. In the rest frame of the heavy quark, only the temporal component of the following bilinear is important at $1/m_b$ order

$$\frac{1}{m_b^2} (\bar{b}^\alpha \bar{D}_\rho \Gamma D^\rho s^\alpha) = \pm \frac{1}{m_b} (\bar{b}^\alpha \Gamma D^0 s^\alpha) + \mathcal{O}\left(\frac{1}{m_b^2}\right) \quad (3)$$

where the sign is determined by whether the temporal derivative acts on an outgoing heavy quark or an incoming heavy antiquark. Γ represents either $\gamma^\mu (1 - \gamma^5)$ (R_2) or $1 - \gamma^5$ (R_3). Using the equation of motion for the strange quark, and neglecting contributions of $\mathcal{O}(m_s/m_b)$, $\hat{R}_{2,3} = \pm (1/m_b) (\bar{b}^\alpha \Gamma \gamma_0 \boldsymbol{\gamma} \cdot \mathbf{D} s^\alpha) (\bar{b}^\beta \Gamma s^\beta)$, and similarly for $\hat{\tilde{R}}_{2,3}$. In order to implement the derivative operator, the calculation of the associated three-point correlation functions will require new strange quark propagators, beyond those used in Ref. [6], with point-split inversion sources at

the operator location. We use a symmetric difference operator in each of the spatial dimensions as the source for the inversion of the HISQ Dirac matrix on Coulomb-gauge-fixed configurations. Note we use a hat on an operator when we wish to call attention to the 4-quark operator computed directly on the lattice, in distinction to a linear combination such as a renormalized, matched, or subtracted operator.

As discussed below, we will also need matrix elements of the dimension-6 operators \hat{O}_1 and \hat{O}_2 . At no additional cost, we recompute these here and check that they agree with the high-statistics study [6].

Matrix elements are obtained from fits to two- and three-point correlation functions using methods developed in Refs. [6,24–26]. Some details have appeared in Ref. [27].

The prediction of a matrix element of a higher dimension operator using lattice NRQCD is complicated by mixing with lower dimension operators [28]. The presence of the lattice cutoff a means that the matrix elements $\langle \hat{R}_{2,3} \rangle$ will contain contributions from $\langle \hat{O}_{1,2} \rangle$ of the order $\mathcal{O}(\alpha_s/(am_b))$. We have used lattice perturbation theory to calculate the coefficients ξ_{ij} which parametrize this mixing at one-loop level. Matrix elements of the subtracted operator,

$$R_i^{\text{sub}} = \hat{R}_i - \alpha_V \xi_{ij} \hat{O}_j \quad (4)$$

will have power-law mixing canceled through $\mathcal{O}(\alpha_s)$. The coefficients ξ_{ij} have not been calculated before. The procedure is a straightforward extension of Ref. [29], in particular Sec. IV. B. In this instance the derivative acts on the light quark propagator instead of the heavy quark propagator. Numerical values are tabulated in Table I. For the strong coupling constant, we use $\alpha_V(2/a)$ (see Table I of Ref. [30], inferred from the work of [31,32]). Using $\alpha_{\overline{\text{MS}}}(m_b)$ [5] in Eq. (4) does not significantly affect our final results.

Figure 1 illustrates the effect of the subtraction Eq. (4). Matrix elements of \hat{R}_i and R_i^{sub} are shown normalized to $\langle O_1 \rangle$ [6]. The fact that the matrix element of the subtracted operator is 50% (R_2) to 70% (R_3) of the unsubtracted operator shows that this subtraction is significant. This is of comparable size to the effects seen in the $1/m_b$ contributions to the B and B_s decay constants [28,33] and matrix

TABLE I. Perturbative coefficients used in Eq. (4) for the values of am_b used on each ensemble, very coarse (VC), coarse (C), and fine (F) spacing with $m_s/m_l = 5$ or physical (p).

Coeff	VC5	VCp	C5	Cp	F5
ξ_{21}	-0.1311	-0.1327	-0.1557	-0.1573	-0.2004
ξ_{22}	0.0092	0.0093	0.013	0.0133	0.0225
ξ_{31}	-0.0331	-0.0334	-0.0392	-0.0397	-0.0508
ξ_{32}	-0.2829	-0.2864	-0.3404	-0.3449	-0.451

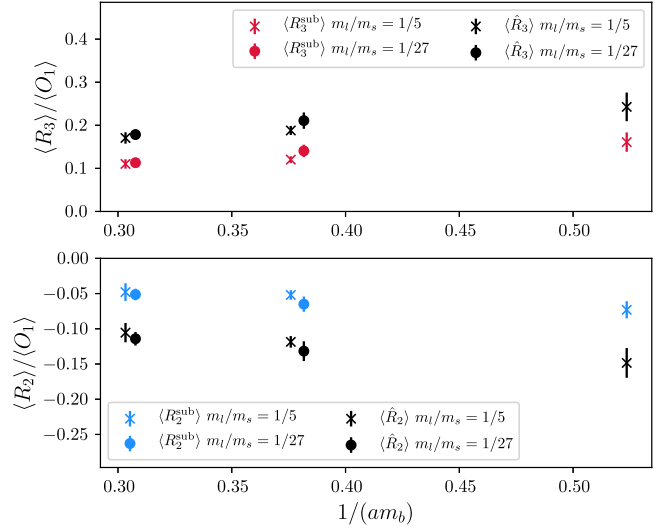


FIG. 1. Ratios of unsubtracted and subtracted R matrix elements to $\langle O_1 \rangle$. Only statistical errors are shown here.

elements $\langle O_j \rangle$ [34]. Figure 1 shows that, as expected, the subtraction leads to a reduction in a dependence over the range of lattice spacings used.

We must estimate the uncertainty due to not knowing the $\mathcal{O}(\alpha_s)$ $\overline{\text{MS}}$ -to-lattice matching of the R operators nor the $\mathcal{O}(\alpha_s^2)$ contributions from the dimension-6 operators. Both of these are suppressed by a power of α_s compared to matrix elements of the two terms in Eq. (4). Therefore, we include these truncation errors in our results by multiplying our results by a noisy estimator $\langle R_i \rangle = \langle R_i^{\text{sub}} \rangle (1 + \alpha_V \delta_{am_b})$, where $\delta_{am_b} = 0 \pm 1$ is a Gaussian-distributed random variable, one for each of the three lattice spacings. This is our largest source of uncertainty.

Our calculations include numerical data obtained with all quark masses tuned close to their physical values. In order to include some data with unphysically large values for the up and down sea quark masses, we assume an analytic dependence on these masses. We also parametrize discretization errors, e.g., due to the gluon and staggered fermion actions, in powers of $(a\Lambda_{\text{QCD}})^2$ taking $\Lambda_{\text{QCD}} = 500$ MeV. Results presented here come from fits to

$$\frac{\langle R_j \rangle}{f_{B_s}^2 M_{B_s}^2} = \beta [1 + d_2 (a\Lambda_{\text{QCD}})^2 + d_4 (a\Lambda_{\text{QCD}})^4 + c_1^{s,\text{val}} x_s + c_1^{\text{sea}} (2x'_\ell + x'_s)] \quad (5)$$

where sea quark mass dependence is parametrized by $x'_\ell = M_\pi^2 / (2\Lambda_\chi)^2$ and $x'_s = (2M_K^2 - M_\pi^2) / (2\Lambda_\chi)^2$, with $\Lambda_\chi = 1$ GeV. We use the lattice masses aM_π and aM_K tabulated in Ref. [17]. For the valence strange quark $x_s = M_{\eta_s}^2 / (2\Lambda_\chi)^2$, the η_s being a fictitious flavor-nonsinglet $\bar{s}s$ pseudoscalar meson, which is nevertheless well defined in chiral perturbation theory. Values for aM_{η_s}

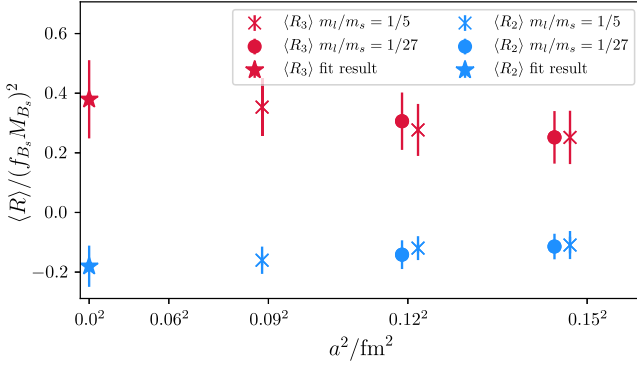


FIG. 2. Matrix elements of R_2 and R_3 plotted against lattice spacing squared. Error bars include systematic uncertainties. Results of fits to Eq. (5) are plotted as stars.

on these ensembles [35] are used to parametrize the difference between the input valence strange quark mass and the physical one, using for the “physical” value $M_{n_s} = 688.5(2.2)$ MeV [35,36]. We assume Gaussian priors of 0 ± 1 for the fit parameters, except for d_2 , which we take to be 0 ± 5 . In the fits, we find $|d_2| \approx 2.5 \pm 2.0$.

As one would expect, any sensitivity of the $B_s - \bar{B}_s$ matrix elements to the light sea quark mass is much smaller than our uncertainties. The slight mistunings in the sea or valence strange quark masses are not large enough to give a nonzero result for c_1^s parameters. Including terms that are quadratic in the x variables has no effect on the fit. Similarly, we obtain d_4 consistent with zero. Within errors the data is consistent with a mild a^2 dependence (see Fig. 2).

Our main results are for the pair of matrix elements

$$\langle B_s | R_2 | \bar{B}_s \rangle = -(0.18 \pm 0.07) f_{B_s}^2 M_{B_s}^2 \quad (6)$$

$$\langle B_s | R_3 | \bar{B}_s \rangle = (0.38 \pm 0.13) f_{B_s}^2 M_{B_s}^2 \quad (7)$$

or for the linearly dependent, color-rearranged operator matrix elements [Eq. (2)]

$$\langle B_s | \tilde{R}_2 | \bar{B}_s \rangle = (0.18 \pm 0.07) f_{B_s}^2 M_{B_s}^2 \quad (8)$$

$$\langle B_s | \tilde{R}_3 | \bar{B}_s \rangle = (0.29 \pm 0.10) f_{B_s}^2 M_{B_s}^2. \quad (9)$$

At the accuracy with which we work, these results can be interpreted as the $\overline{\text{MS}}$ -scheme results at the scale $\mu_2 = m_b$, with an uncertainty included to account for the fact that the lattice-continuum matching is tree level.

It is sometimes convenient to include a numerical factor which arises from the vacuum saturation approximation (VSA). We define B' factors via $\langle B_s | R_k | \bar{B}_s \rangle = q f_{B_s}^2 M_{B_s}^2 B'_{R_k}$ where q is $-\frac{2}{3}$, $\frac{2}{3}$, $\frac{7}{6}$, and $\frac{5}{6}$ for R_2 , \tilde{R}_2 , R_3 , and \tilde{R}_3 , respectively. The “unprimed” bag factors B_{R_k} which are equal to 1 in the VSA include a mass factor such that $B'_{R_k} = [M_{B_s}^2 / (m_b^{\text{pow}})^2 - 1] B_{R_k}$ [1]. These B_{R_k} are the ones taken in

TABLE II. Results for bag factors of operator labeled by k . The right column uses $M_{B_s} = 5.36688(17)$ GeV [37] and $m_b^{\text{pow}} = 4.70(10)$ GeV [13].

k	B'_{R_k}	B_{R_k}	k	B'_{R_k}	B_{R_k}
R_2	0.27(10)	0.89(38)	\tilde{R}_2	0.27(10)	0.89(38)
R_3	0.33(11)	1.07(42)	\tilde{R}_3	0.35(13)	1.14(46)

recent phenomenological estimates [2,11,13] to be 1.0 ± 0.5 in the absence of a QCD calculation. We tabulate numerical results of our work in Table II. It turns out that the VSA expectation is a reasonable back-of-the-envelope estimate, although it must be emphasized that this agreement is very sensitive to the arbitrary definition of m_b^{pow} — even the 2% uncertainty quoted in m_b^{pow} leads to an 18% uncertainty in B'_{R_k}/B_{R_k} . (Note that the B' factors do not depend on m_b^{pow} .) Our results replace the rough VSA estimates with a lattice QCD computation where all uncertainties are quantified.

The matrix elements determined in Ref. [6] allow determination of the remaining 3 matrix elements $B'_{R_0} = -\frac{3}{4} \langle B_s | R_0 | \bar{B}_s \rangle / (f_{B_s} M_{B_s})^2 = 0.32(13)$, $B'_{R_1} = \frac{3}{7} \langle B_s | O_4 | \bar{B}_s \rangle / (f_{B_s} M_{B_s})^2 = 1.564(64)$, and $B'_{\tilde{R}_1} = \frac{3}{5} \langle B_s | O_5 | \bar{B}_s \rangle / (f_{B_s} M_{B_s})^2 = 1.167(46)$.

Our results permit the first lattice determination of $\Delta\Gamma_{1/m_b}$, the power-law corrections to $\Delta\Gamma_s$. Recently there has been an investigation of scale and scheme dependence of the leading term in $\Delta\Gamma_s$, where it has been proposed to include corresponding uncertainties as follows [14]:

$$\Delta\Gamma_s = [1.86(17)B_1 + 0.42(3)B'_3] f_{B_s}^2 + \Delta\Gamma_{1/m_b} \quad (10)$$

in the $\overline{\text{MS}}$ scheme. Taking $f_{B_s} = 0.2307(12)$ GeV from Ref. [38] and weighted averages of $B_1 = 0.84(3)$ and $B'_3 = 1.36(8)$ from Refs. [5,6] yields a result for the leading order contribution, $\Delta\Gamma_s^{\text{LO}} = 0.114(9)$ ps $^{-1}$.

The $1/m_b$ contribution to $\Delta\Gamma_s$ can be expressed as a linear combination of the matrix elements of the R operators, times perturbative coefficients γ_k [1,13]. Writing $\Delta\Gamma_{1/m_b} = -2\tilde{\Gamma}_{12,1/m_b} \cos\phi_{12}$, we have

$$\tilde{\Gamma}_{12,1/m_b} = \frac{G_F^2 f_{B_s}^2 M_{B_s} m_b^2}{24\pi} \sum_k \gamma_k(\bar{z}) B'_{R_k}. \quad (11)$$

Here k is an index that runs over the four operators in Eq. (1) plus the three color-rearranged operators. The $\gamma_k(\bar{z})$ are related to the $g_k(\bar{z})$ of [13] by the numerical coefficients relating the matrix elements to the B' factors; additionally γ_1 and $\tilde{\gamma}_1$ include a factor of $\bar{m}_s(\bar{m}_b)/\bar{m}_b(\bar{m}_b)$. The functions $g_k(\bar{z})$ depend on $\bar{z} = [\bar{m}_c(\bar{m}_b)/\bar{m}_b(\bar{m}_b)]^2$ [39] and the leading order $H^{\Delta F=1}$ Wilson coefficients $C_1^{(0)}$ and

$C_2^{(0)}$. Numerical values used here are given in Supplemental Material [20]. Only the terms with B'_{R_0} , B'_{R_2} , and $B'_{\bar{R}_2}$ contribute to $\Delta\Gamma_{1/m_b}$ due to the smallness of the other γ_k .

Our result for Eq. (11) is $\tilde{\Gamma}_{12,1/m_b} = 0.0110(52) \text{ ps}^{-1}$ which, given $\cos\phi_{12} = 1$ to the precision relevant here, contributes to the width difference as

$$\Delta\Gamma_{1/m_b} = -2\tilde{\Gamma}_{12,1/m_b} = -0.022(10) \text{ ps}^{-1}. \quad (12)$$

The uncertainty in Eq. (12) is dominated by that of $\langle\tilde{R}_2\rangle$. From studies of the leading $\Delta\Gamma_s$ term, we expect scale and scheme uncertainties here to similarly be at the 10% level, i.e., not significant compared to the present hadronic uncertainty.

Combining Eq. (12) with Eq. (10), we find

$$\Delta\Gamma_s = 0.092(14) \text{ ps}^{-1}. \quad (13)$$

The error in Eq. (13) is mostly due to the uncertainty in $\Delta\Gamma_{1/m_b}$; its variance contributes approximately 60% to the total variance in Eq. (13). The next largest uncertainty, contributing 30%, comes from the coefficients in the first term of Eq. (10). The variance of B_1 contributes 8% of the total.

The HFLAV Collaboration average of experimental measurements is $\Delta\Gamma_s = 0.085(6) \text{ ps}^{-1}$ [40]. This is in good agreement with our result [Eq. (13)] with half the uncertainty.

There remains more to do in order for the theoretical prediction to match the experimental precision. The next generation lattice calculation will require one-loop matching of lattice to $\overline{\text{MS}}$ regularization schemes in order to reduce the uncertainty in $\Delta\Gamma_{1/m_b}$. At the same time the work to determine the perturbative coefficients appearing in Eq. (10) through NNLO must be completed. First steps have already begun [14].

We thank the MILC Collaboration for their gauge configurations and their code MILC-7.7.11 [41]. M. W. is grateful for an IPPP Associateship held while some of this work was undertaken and for discussions with A. Lenz. This work was funded in part by the STFC, the NSF, and the DOE. C. J. M. is supported in part by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under Contracts No. DE-FG02-00ER41132 and No. DE-AC05-06OR23177. Results described here were obtained using the Darwin Supercomputer of the University of Cambridge High Performance Computing Service as part of the DiRAC facility jointly funded by STFC, the Large Facilities Capital Fund of BIS and the Universities of Cambridge and Glasgow.

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