High-precision f_{B_s} and heavy quark effective theory from relativistic lattice QCD

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We present a new determination of the B_s leptonic decay constant from lattice QCD simulations that use gluon configurations from MILC and a highly improved discretization of the relativistic quark action for both valence quarks. Our result, $f_{B_s} = 0.225(4)$ GeV, is almost 3 times more accurate than previous determinations. We analyze the dependence of the decay constant on the heavy quark's mass and obtain the first empirical evidence for the leading $1/\sqrt{m_h}$ dependence predicted by heavy quark effective theory. As a check, we use our analysis technique to calculate the $m_{B_s} - m_{\eta_b}/2$ mass difference. Our result agrees with experiment to within errors of 11 MeV (better than 2%). We discuss how to extend our analysis to other quantities in B_s and B physics, making 2% precision possible for the first time.

Lattice simulations of QCD have become essential for high-precision experimental studies of B-meson decays—studies that test our understanding and the limitations of the standard model of weak, electromagnetic and strong interactions, and also determine fundamental parameters, like the Cabibbo-Kobayashi-Maskawa matrix, in that model. Accurate theoretical calculations of QCD contributions to meson masses, decay constants, mixing amplitudes, and semileptonic form factors are critical for this program, and lattice simulation is the main tool for providing these calculations. A major complication for the lattice simulations has been the large mass of the b quark, which has necessitated the use of nonrelativistic effective field theories like nonrelativistic QCD (NRQCD) to describe b dynamics in the simulations. The need for effective field theories has made it difficult to achieve better than 5–10% precision for many important quantities.

Recently we overcame the analogous problem for c quarks by introducing a highly improved discretization of the relativistic quark action that gives accurate results even on quite coarse lattices: the highly improved staggered-quark (HISQ) discretization [1]. With this formalism, c quarks are analyzed in the same way as u, d, and s quarks, which greatly reduces the uncertainties in QCD simulations of D physics [2–7]. More recently we showed that the HISQ action can be pushed to much higher masses—indeed, very

close to the b mass—using new lattices, from the MILC Collaboration, with the smallest lattice spacing available today ($a = 0.044$ fm). This allowed us to extract a value for the b's $\overline{MS}$ mass that was accurate to better than 1%. Here we extend that work in a new analysis of the B_s meson's leptonic decay constant f_{Bs}, which produces the most accurate theoretical value to date.

We also compute the mass difference $m_{B_s} - m_{\eta_b}/2$, as an additional test of our analysis method. This difference is particularly sensitive to QCD dynamics because the leading (and uninteresting) dependence on the heavy quark's mass mostly cancels in the difference.

It would be quite expensive to extend our new analysis directly to B-meson quantities, because of the added costs associated with very light valence and sea quarks. This is unnecessary, however, because heavy-quark effective field theories like NRQCD already give accurate results for ratios of B_s to B quantities, like f_{B_s}/f_B. This is because the largest systematic errors from these effective theories, due to operator matching, cancel in such ratios. The ratio of the decay constants, for example, is known to $\pm 2\%$ from effective field theories [8]. So the combination of accurate B_s quantities from HISQ simulations, as discussed in this paper, with B_s/B ratios from NRQCD or other effective field theories provides a potent new approach to high-precision b physics generally. Note that no operator matching is required in our relativistic analysis of f_{B_s} because of the exact chiral symmetry of the HISQ formalism in the massless limit.

In our simulations for this paper, we computed decay constants and masses for nonphysical H_s mesons composed of an s quark, and heavy quarks h with various masses m_h ranging from below the c mass to just below the b mass. This data allows us to extrapolate to the b mass,

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TABLE I.   Parameter sets used to generate the 3-flavor gluon configurations analyzed in this paper. The lattice spacing is specified in terms of the static-quark potential parameter $r_1 = 0.3133(23)$ fm [10]; values for r_1/a are from [9]. The bare quark masses are for the asqtad formalism[9] used for the sea quarks and u_0 is the fourth root of the plaquette. The spatial (L) and temporal (T) lengths of the lattices are also listed, as are the number of gluon configurations (N_{cf}) and the number of time sources (N_{ts}) per configuration used in each case.

Set	r_1/a	$au_0m_{0u/d}$	au_0m_{0s}	u_0	L/a	T/a	$N_{cf} \times N_{ts}$
1	2.152(5)	0.0097	0.0484	0.860	16	48	631×2
2	2.618(3)	0.01	0.05	0.868	20	64	595×2
3	3.699(3)	0.0062	0.031	0.878	28	96	566×4
4	5.296(7)	0.0036	0.018	0.888	48	144	201×2
5	7.115(20)	0.0028	0.014	0.895	64	192	208×2

where $m_{H_s} = m_{B_s}$. We repeated our analysis for five different lattice spacings, allowing us also to extrapolate our results to zero lattice spacing.

The gluon configuration sets we used are from the MILC Collaboration [9] and are described in Table I. Our simulation results for the decay constants and meson masses, for various values of the h mass, are presented in Table II. We also give results for the mass of the pseudoscalar $h\bar{h}$ meson, m_{η_h}, and for the mass of the η_s meson. The η_s is an unphysical pseudoscalar $s\bar{s}$ meson whose valence quarks are not allowed to annihilate; we use its mass to tune the bare mass of the s quark: simulations show that its mass is $m_{\eta_s,\text{phys}} = 0.6858(40)$ GeV when the s mass is correctly tuned [10].

We expect some statistical correlation between results from the same configuration set but with different h-quark masses. We have not measured this, but we have verified that our results are insensitive (at the level of $\pm\sigma/4$) to such correlations. We introduce a 50% correlation for our fits, which increases our final error estimates slightly.

Our strategy for extracting f_{B_s} is first to fit our simulation results for f_{H_s} to the HQET-inspired formula [11]

$$f_{H_s}(a, m_{H_s}, m_{\eta_s}) = A(m_{H_s})^b \left(\frac{\alpha_V(m_{H_s})}{\alpha_V(m_{D_s})} \right)^{-2/\beta_0}$$

$$\times \sum_{i=0}^{N_m-1} C_i(a) \left(\frac{1}{m_{H_s}} \right)^i + c_s(m_{\eta_s}^2 - m_{\eta_s,\text{phys}}^2),$$

$$(1)$$

where $\beta_0 = 11 - 2n_f/3 = 9$ in our simulations [12], α_V is the QCD coupling in the V scheme [5,13], and constant $b = -0.5$ from HQET. We use m_{H_s} as a proxy for the h-quark mass since its value for b quarks is known from experiment. All masses in this formula are in GeV units, so the expansion under the sum is in powers of $(1\text{ GeV})/m_{H_s}$. The prior value on the overall constant A is taken to be very broad: 0 ± 2. The last term in Eq. (1) corrects for tuning errors in the s-quark mass; we determined that $c_s = 0.06(1)$ by repeating our calculations with slightly different s masses [14]. We parameterize the term which accounts for lattice spacing dependence as

$$C_i(a) = \sum_{j,k,l=0}^{N_a-1} c_{ijkl} \left(\frac{am_h}{\pi} \right)^{2j} \left(\frac{am_s}{\pi} \right)^{2k} \left(\frac{a\Lambda_{\text{QCD}}}{\pi} \right)^{2l} \quad (2)$$

TABLE II.   Simulation results for each of the five configuration sets (Table I) and several values of the heavy-quark's mass m_h. The s-quark's mass m_s is tuned to be close to its physical value. Results are given for: the leptonic decay constant f_{H_s} and mass m_{H_s} of the pseudoscalar $h\bar{s}$ meson, and masses of the pseudoscalar $h\bar{h}$ and $s\bar{s}$ mesons, m_{η_h} and m_{η_s}, respectively.

|	am_s	am_{η_s}	am_h	am_{H_s}	af_{H_s}	am_{η_h}
1	0.061	0.5049(4)	0.66	1.3108(6)	0.1913(7)	1.9202(2)
	0.061	0.5049(4)	0.81	1.4665(8)	0.197(1)	2.1938(2)
2	0.0492	0.4144(2)	0.44	0.9850(4)	0.1500(5)	1.4240(1)
	0.0492	0.4144(2)	0.63	1.2007(5)	0.1559(7)	1.8085(1)
	0.0492	0.4144(2)	0.85	1.4289(8)	0.161(1)	2.2193(1)
3	0.0337	0.2941(1)	0.3	0.7085(2)	0.1054(2)	1.03141(8)
	0.0337	0.2941(1)	0.413	0.8472(2)	0.1084(2)	1.28057(7)
	0.0337	0.2941(1)	0.7	1.1660(4)	0.1112(5)	1.86536(5)
	0.0337	0.2941(1)	0.85	1.3190(5)	0.1123(6)	2.14981(5)
4	0.0228	0.2062(2)	0.273	0.5935(2)	0.0750(3)	0.8994(1)
	0.0228	0.2062(2)	0.564	0.9313(5)	0.0754(6)	1.52542(6)
	0.0228	0.2062(2)	0.705	1.0811(8)	0.0747(8)	1.80845(6)
	0.0228	0.2062(2)	0.85	1.228(1)	0.074(1)	2.08753(6)
5	0.0165	0.1548(1)	0.195	0.4427(3)	0.0555(3)	0.67113(6)
	0.0165	0.1548(1)	0.5	0.8038(8)	0.055(1)	1.34477(8)
	0.0165	0.1548(1)	0.7	1.017(1)	0.053(2)	1.75189(7)
	0.0165	0.1548(1)	0.85	1.168(2)	0.052(2)	2.04296(7)
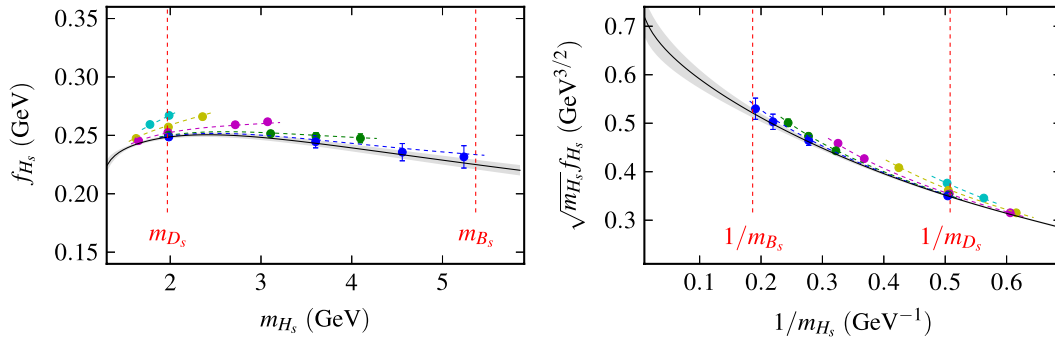
FIG. 1 (color online). The leptonic decay constant f_{H_s} for pseudoscalar $h\bar{s}$ mesons H_s, plotted on the left versus the H_s mass as the h-quark's mass is varied. The solid line and gray band show our best-fit estimates for the decay constants extrapolated to zero lattice spacing. Best-fit results (dashed lines) and simulation data are also shown for five different lattice spacings, with results for smaller lattice spacings extending to higher masses (since we restrict $am_h < 1$). The simulation data points have been corrected for small mistunings of the s quark's mass. On the right the same simulation data and fits are plotted for $\sqrt{m_{H_s}}f_{H_s}$ versus $1/m_{H_s}$.

with $N_m = N_a = 4$ [15]. We choose $c_{0000} = 1$. This expansion is in powers of quark masses and the QCD scale parameter $\Lambda_{QCD} \approx 0.5$ GeV divided by the ultraviolet cut-off for the lattice theory: $\Lambda_{UV} \approx \pi/a$. The fit parameters are the coefficients c_{ijkl} for each of which we use a prior of 0 ± 1.5, which is conservative [16]. The lattice spacing effects are dominated by the am_h terms. We include both am_s and $a\Lambda_{QCD}$ for completeness, but they have a very small effect because a is small for most of our data. Leaving out either or both makes no difference to our results.

Our data for five different lattice spacings and a wide range of masses m_{H_s} are presented with our fit results in Fig. 1. The reach in m_{H_s} grows as the lattice spacing decreases (since we restrict $am_h < 1$), and deviations from the continuum curve get smaller. The fit is excellent, with a χ^2 per degree of freedom of 0.36 while fitting all 17 measurements. The small χ^2 results from our conservative priors (we get excellent fits and smaller errors with priors that are half the width).

Having determined the parameters in Eq. (1), the second step in our analysis is to set $M_{H_s} = M_{B_s}$, $a = 0$, and $m_{\eta_s} = m_{\eta_s,phys}$ in that formula to obtain our final value for f_{B_s},

$$f_{B_s} = 0.225(4) \text{ GeV}, \qquad (3)$$

which agrees well with the previous best NRQCD result of 0.231(15) GeV [17] but is almost 4 times more accurate. Our result also agrees with the recent result of 0.232 (10) GeV from the ETM Collaboration, although that analysis includes only two of the three light quarks in the quark sea [18]. Two additional new results, both using effective field theories for the b dynamics and both with three flavors of sea quarks were announced at *Lattice 2011* [8]: 0.226(10) GeV from the HPQCD Collaboration and 0.242(10) GeV from the Fermilab Lattice/MILC Collaboration.

Our total error is split into its component parts following the procedure described in [19] to give the error budget in Table III. It shows that the dominant errors come from statistical uncertainties in the simulations, the $m_{H_s} \to m_{B_s}$ extrapolation, the $a^2 \to 0$ extrapolation, and uncertainties in the scale-setting parameter r_1. Our analysis of f_{D_s} in [6] indicates that finite volume errors, errors due to mistuned sea-quark masses, errors from the lack of electromagnetic corrections, and errors due to lack of c quarks in the sea are all significantly less than 1%, and so negligible compared with our other uncertainties. Our final result is also insensitive to the detailed form of the fit function; for example, doubling the number of terms has negligible effect (0.03σ) on the errors and value.

We have also included in Fig. 1 (right) a plot of $\sqrt{m_{H_s}}f_{H_s}$ for different values of m_{H_s}. This shows that there are large nonleading terms in f_{H_s}, beyond the leading $1/\sqrt{m_{H_s}}$ behavior predicted by HQET. Our simulation nevertheless provides evidence for the leading term. Treating exponent b in Eq. (1) as a fit parameter, rather than setting it equal to

TABLE III. Dominant sources of uncertainty in our determinations of the B_s decay constant and the $B_s - \eta_b$ mass difference. Contributions are shown from the extrapolations in m_{H_s}, a^2 and m_s, as well as statistical errors in the simulation data and errors associated with the scale-setting parameter r_1. Other errors are negligible.

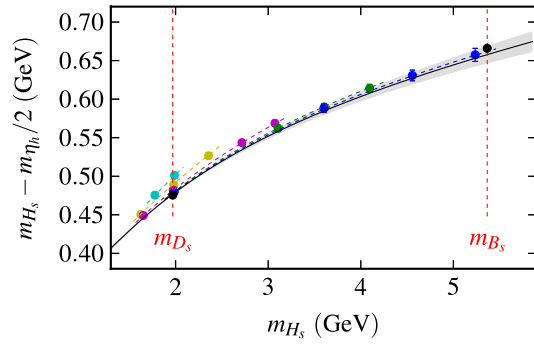|	f_{B_s}	$m_{B_s} - m_{\eta_b}/2$
Monte Carlo statistics	1.30%	1.49%
$m_{H_s} \to m_{B_s}$ extrapolation	0.81	0.05
r_1 uncertainty	0.74	0.33
$a^2 \to 0$ extrapolation	0.63	0.76
$m_{\eta_s} \to m_{\eta_s,phys}$ extrapolation	0.13	0.18
r_1/a uncertainties	0.12	0.17
Total	1.82%	1.73%

FIG. 2 (color online). The $H_s - \eta_h/2$ mass difference plotted versus m_{H_s} as the h quark's mass is varied. The solid line and gray band show our best-fit estimates for the mass differences extrapolated to zero lattice spacing. Best-fit results (dashed lines) and simulation data are also shown for five different lattice spacings, with results for smaller lattice spacings extending to larger masses (since we require $am_h < 1$). The simulation data points have been corrected for small mistunings in the s quark's mass. Data points (in black) at m_{D_s} and m_{B_s} are the experimental values after correcting for small effects from electromagnetism, η_b annihilation, and c quarks in the sea, none of which are included in the simulation.

-0.5, we find a best-fit value of $b = -0.51(13)$, in excellent agreement with the HQET prediction. This is the first empirical evidence for this behavior.

Our analysis also yields a value for f_{D_s}, which agrees with [6]. It is also clear from Fig. 1 (left) that f_{H_s} peaks between f_{D_s} and f_{B_s}, and that f_{B_s} is smaller—we find:

$$f_{B_s}/f_{D_s} = 0.906(14). \tag{4}$$

HQET suggests a ratio less than one, but previous lattice QCD results have been ambiguous about this point.

To check our f_{B_s} analysis technique, we adapted the same technique to compute the mass difference [20]

$$\Delta \equiv m_{H_s} - m_{\eta_h}/2, \tag{5}$$

using, as inputs, the masses m_{η_h} computed in our simulations for pseudoscalar $h\bar{h}$ mesons made of our heavy quark. Our values for Δ come from the results in Table II. We fit them to

$$\Delta(a, m_{H_s}, m_{\eta_s}) = A_m(m_{H_s})^{b_m} \sum_{i=0}^{N_m-1} D_i(a)\left(\frac{1}{m_{H_s}}\right)^i$$
$$+ d_s(m_{\eta_s}^2 - m_{\eta_s,\text{phys}}^2) \tag{6}$$

where our simulations indicate that $d_s = 0.18(1)$, and we take $b_m = 1$ because of the η_h binding energy [21]. $D_i(a)$ has an expansion similar to that for $C_i(a)$ [Eq. (2)], with the same priors and A_m has the same prior as A.

We show the best fit to our simulation data in Fig. 2. Again, the fit is excellent, which a χ^2 per degree of freedom of 0.13 while fitting all 17 measurements.

Extrapolating to the b mass, we obtain our best-fit value for the mass splitting,

$$m_{B_s} - m_{\eta_b}/2 = 0.658(11) \text{ GeV}, \tag{7}$$

which agrees well with experiment: experiment gives 0.671(2) GeV which becomes 0.666(4) after removing corrections from electromagnetism, η_b annihilation, and c quarks in the sea (not included in our simulations) [20,22]. Our fit also gives a value for $m_{D_s} - m_{\eta_c}/2$; it also agrees well with experiment [6].

In this paper, we have shown how to use a highly improved discretization of the relativistic quark action to make accurate calculations for mesons containing b quarks. Our result for the B_s decay constant, $f_{B_s} = 0.225(4)$ GeV, agrees with other determinations from lattice QCD but is almost 3 times more accurate than the most precise previous result. The reliability of our extrapolations is underscored both by our previous determination of the b-quark's $\overline{\text{MS}}$ mass, which agrees with other determinations to within errors of less than $\pm 1\%$, and by our calculation here of the $m_{B_s} - m_{\eta_b}/2$ mass difference, which agrees with experiment to within errors of ± 11 MeV or less than 2%. Our analysis of the decay constant gives the most extensive information to date on the heavy-quark mass dependence of the decay constant, and provides the first empirical evidence for the leading $1/\sqrt{m_h}$ dependence predicted by HQET. Further results on the B_c mesons, and the decay constant f_{η_h} will be presented elsewhere [23].

Our analysis has important implications for future lattice simulations of B physics. Other B_s quantities, like semileptonic form factors, can be analyzed in the same way, bringing few-percent precision within reach. Similar precision for B quantities is possible by combining B_s calculations like these with precise calculations of B_s/B ratios using (very efficient) nonrelativistic effective field theories for b-quark dynamics.

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[11] For a review of HQET and its application to f_{B_s} see G. Buchalla, in *The Proceedings of the 55th Scottish Universities Summer School in Physics* edited by C. T. H. Davies and S. M. Playfer (IOP, Bristol, 2002).

[12] We include only the leading-order anomalous dimension because of the limited precision of our data. Our results are essentially unchanged if we omit leading order as well.

[13] C. T. H. Davies *et al.* (HPQCD Collaboration), Phys. Rev. D **78**, 114507 (2008).

[14] Parameter c_s depends upon M_{H_s} but we have verified that such variation has negligible impact on our analysis given our statistical errors. Our value for c_s agrees with the f_{D_s} slope given in [6].

[15] We are able to fit this (large) number of parameters because we use a Bayesian fit in which each parameter is given a prior value. The prior values are incorporated into the fit's χ^2 function in such a way that each counts as an additional piece of input data. As a result, the number of degrees of freedom in the fit always equals the number of pieces of original Monte Carlo data, however many parameters there are. Adding terms to the fit function that are not needed can only increase the final errors. We include such terms to make sure that our systematic errors are not underestimated. Generally, we add terms at least until the fit results and χ^2 stop changing. For more details see: G. P. Lepage *et al.*, Nucl. Phys. B, Proc. Suppl. **106**, 12 (2002).

[16] Naively one expects $c_{ijkl} \approx O(1)$. The empirical Bayes criterion, for example, indicates that a prior of 0 ± 1 is optimal. Making the prior 50% wider is conservative and increases our final error estimates. We also checked our choice of expansion parameter for the am_h expansion using this criterion. Assuming $c_{ijkl} = 0 \pm 1$, the empirical Bayes criterion indicates that the optimal expansion parameter is $1.2am_h/\pi$ rather than am_h/π. This choice of prior and expansion parameter gives the same answers but with slightly smaller errors than the result given here. The empirical Bayes criterion is discussed in the reference in [15]. We have also tested even larger expansion parameters such as $1.4am_h/\pi$ with the same results. This demonstrates the robustness of the fit.

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[21] Our value for slope d_s agrees reasonably well with the value 0.20(1) found for m_{D_s} in [6]. Treating exponent b_m as a fit parameter with a broad prior (1(1)) results in a value of $b_m = 1.17(47)$, which agrees well with our theoretical expectation ($b_m = 1$).

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