I. INTRODUCTION

Lattice studies of the hadron spectrum provide valuable indications on the reliability of effective field theories. A phenomenologically relevant example is given by effective field theories for heavy quarks, such as heavy quark effective theory (HQET) or nonrelativistic QCD (NRQCD). In this respect, hyperfine splittings are of great theoretical interest, since they vanish in the static limit, and thus serve to probe subleading terms in the heavy quark expansion.

Regarding specifically the hyperfine splitting of the B spectrum, it is well known that the masses of the pseudo-scalar \( B_s \) and vector \( B_s' \) differ as a result of spin effects [1]. This mass difference is produced in HQET by a \( O(1/m_b) \) chromomagnetic term in the Lagrangian that breaks the heavy quark spin symmetry of the static theory [2,3]. In the context of lattice NRQCD it was found that in order to obtain a determination of the hyperfine splittings of bottomonium that is consistent with experiments, the perturbative improvement of the NRQCD action to at least one-loop order is required [4–6], for values of the lattice spacing of about 0.1 fm. The \( \Upsilon \) spectrum, on the other hand, is well reproduced within NRQCD, and has been used in the literature as a quantity to set the lattice spacing [7,8]. Hyperfine splittings have also been studied within the HISQ approach to heavy quarks [9].

In contrast to other studies, our results are based on nonperturbatively renormalized HQET including the next-to-leading order terms in the inverse heavy quark mass expansion. When formulated with a lattice regulator, the resulting lattice field theory can be nonperturbatively matched to QCD in the continuum limit. This provides a rigorous and systematically improvable approach to the study of the B-meson system.

Although permil precision seems difficult to reach within this approach, as it would require including \( 1/m_b^2 \) corrections, the control over systematics such as the nonperturbative subtraction of power divergences and the related existence of the continuum limit, makes the approach very appealing and conceptually sound and in this sense, and in our view, more precise than other methods. In addition, as is evident in [10] and emphasized in [11], for quantities more “complicated” than decay constants, such as form factors, there is great need for results from different approaches, with different levels of control on the various systematics. Applications of the nonperturbative HQET formalism to form factors are well on their way [12–14].
Remaining within spectrum-related observables, another quantity of interest is the SU(3) isospin breaking difference $m_{B_s} - m_B$. Most of the dependence on the heavy quark mass cancels in the difference and the statistical correlations between the strange and light-quark measurements should lead to a much improved precision in the determination of the difference compared to what would be possible for the individual masses. In [15], the mass of the $B_s$-meson has been used to determine the b-quark mass. Since the mass of the $B_s$-meson could have equally possible for the individual masses. In [15], the mass of $B_s$-meson has been used to determine the b-quark mass.

Relatively little is known experimentally on the radial excitations of $B$-mesons, usually denoted by $B''$. CDF has claimed the observation of a resonant state $B(5970)$ that might be identified with radial excitations $B''(5970)$, but, with the exception of the most recent HQET lattice simulations, control of the continuum extrapolation has been limited, if possible at all. An additional difficulty that we observe. They might be identified with radial excitations $B''$, but without a dedicated study including also multihadron operators, we are unable to conclusively determine the nature of these excited states.

In this paper, we report on our estimate of the hyperfine splitting $m_{B''} - m_B$ in the $B$ and $B_s$ systems, and on the mass differences $m_{B''} - m_B$, $m_{B''} - m_B$, and $m_{B''} - m_B$ from $N_f = 2$ lattice simulations.

II. THEORETICAL SETUP

A. HQET on the lattice

The HQET action at $O(1/m_b)$ reads

$$S_{\text{HQET}} = a^4 \sum_x \left\{ \mathcal{L}_{\text{stat}}(x) - \omega_{\text{kin}} \mathcal{O}_{\text{kin}}(x) - \omega_{\text{spin}} \mathcal{O}_{\text{spin}}(x) \right\},$$

where

$$\mathcal{L}_{\text{stat}}(x) = \bar{\psi}(x)D_0 \psi(x),$$

$$\mathcal{O}_{\text{kin}}(x) = \bar{\psi}(x)D^2 \psi(x),$$

$$\mathcal{O}_{\text{spin}}(x) = \bar{\psi}(x)\sigma \cdot B \psi(x),$$

and $\omega_{\text{kin}}$ and $\omega_{\text{spin}}$ are the bare coupling constants for kinetic and spin, respectively.

Table I. Values of HQET parameters at the physical point $\omega(z = z_0)$. As determined in [15], we have used $z_0^{\text{stat}} = 13.24$ to interpolate the parameters of HQET at static order, and $z_0 = 13.25$ for the parameters of HQET expanded to NLO. The bare coupling $g_0$ is given by $\beta = 6/g_0^2$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>HYP1</th>
<th>HYP2</th>
<th>HYP1</th>
<th>HYP2</th>
<th>HYP1</th>
<th>HYP2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$am_{\text{bare}}$</td>
<td>0.969(12)</td>
<td>1.000(12)</td>
<td>1.317(15)</td>
<td>1.350(15)</td>
<td>1.520(17)</td>
<td>1.553(17)</td>
</tr>
<tr>
<td>$am_{\text{bare}}$</td>
<td>0.594(14)</td>
<td>0.606(14)</td>
<td>0.993(17)</td>
<td>1.014(17)</td>
<td>1.214(18)</td>
<td>1.239(18)</td>
</tr>
<tr>
<td>$\omega_{\text{kin}}/a$</td>
<td>0.520(11)</td>
<td>0.525(10)</td>
<td>0.415(8)</td>
<td>0.418(8)</td>
<td>0.377(7)</td>
<td>0.380(7)</td>
</tr>
<tr>
<td>$\omega_{\text{spin}}/a$</td>
<td>0.949(37)</td>
<td>1.090(42)</td>
<td>0.73(28)</td>
<td>0.883(33)</td>
<td>0.655(24)</td>
<td>0.812(30)</td>
</tr>
</tbody>
</table>

B-MESON SPECTROSCOPY IN HQET AT ORDER 1/m

\[ C_{ij}^{\text{stat}}(t) = \sum_{x,y} \mathcal{O}_i(x_0 + t, y) \mathcal{O}_j^*(x) \]  

\[ C_{ij}^{\text{kin/spin}}(t) = \sum_{x,y,z} \mathcal{O}_i(x_0 + t, y, z) \mathcal{O}_j^*(x) \mathcal{O}_{\text{kin/spin}}(z) \]  

containing all pairwise correlators of some set of interpolating fields \( \mathcal{O}_i \), \( i = 1, \ldots, N \), and proceeds to solve the generalized eigenvalue problem (GEVP)

\[ C_{\text{stat}}(t) v_{\text{stat}}^n(t, t_0) = \lambda_{\text{stat}}^n(t, t_0) C_{\text{stat}}(t_0) v_{\text{stat}}^n(t, t_0), \]  

\[ n = 1, \ldots, N, \quad t > t_0. \]  

From the generalized eigenvalues \( \lambda_{\text{stat}}^n(t, t_0) \) and the corresponding eigenvectors \( v_{\text{stat}}^n(t, t_0) \), the effective energy levels can be computed as [34,35]

\[ E_{\text{eff,stat}}^n(t, t_0) = \frac{1}{\lambda_{n}^{\text{stat}}(t, t_0)} \left[ \frac{d}{da} \log \lambda_{n}^{\text{stat}}(t + a, t_0) - \frac{\lambda_{n}^{\text{stat}}(t + a, t_0)}{\lambda_{n}^{\text{stat}}(t, t_0)} \right], \]  

\[ E_{\text{eff,x}}^n(t, t_0) = \frac{\lambda_{n}^{\text{stat}}(t, t_0)}{\lambda_{n}^{\text{stat}}(t, t_0)}, \]  

where \( x \in \{ \text{kin}, \text{spin} \} \) and

\[ \frac{\lambda_{n}^{\text{stat}}(t, t_0)}{\lambda_{n}^{\text{stat}}(t, t_0)} = \frac{v_{\text{stat}}^n(t, t_0)}{v_{\text{stat}}^n(t, t_0)}, \]  

\[ \frac{[\lambda_{n}^{\text{stat}}(t, t_0)]^{-1} C^x(t) - C^x(t_0)}{\lambda_{n}^{\text{stat}}(t, t_0)} v_{\text{stat}}^n(t, t_0). \]  

The corresponding asymptotic behavior is known to be

\[ E_{\text{eff,stat}}^n(t, t_0) = E_{\text{stat}}^n + \beta_{\text{stat}}^{n} e^{-\Delta_{\text{stat}} E_{\text{stat}}^n}, \]  

\[ E_{\text{eff,x}}^n(t, t_0) = E_{\text{stat}}^n + \left[ \beta_{\text{stat}}^{n} + \beta_{\text{kin}}^{n} t \Delta_{\text{stat}} E_{\text{stat}}^n \right] e^{-\Delta_{\text{stat}} E_{\text{stat}}^n}], \]

where the energy gap is defined as \( \Delta_{\text{stat}} E_{\text{stat}}^n = E_n - E_n \).

In our study, the operator basis used is given by heavy-light bilinears with varying levels of Gaussian smearing [36] applied to the light quark field,

\[ O_k(x) = \psi_k(x) \gamma_5 \gamma_q \phi(x), \]  

\[ \psi_q(x) = (1 + k \alpha^2 \Delta) R_1 \phi(x), \]

where \( q = u/d \) or \( s \). The covariant Laplacian \( \Delta \) is built from gauge links that have been triply APE smeared [37,38] in the spatial directions, and the smearing parameters \( k_G \) and \( R_k \) are chosen so as to approximately cover the same sequence of physical radii at each value of the lattice spacing, as discussed in [15]. We solve the GEVP for the matrix of correlators in the static limit for \( N = 3 \).

An illustration of two typical plateaux of the energies \( E_1^{\text{spin}} \) and \( E_2^{\text{stat}} \) is shown in Fig. 1. The plateau regions used for weighted averaging have been chosen by applying the procedure already discussed in [39,40] in order to ensure that the systematic errors due to excited-state contributions are less than a given fraction (typically 1/3) of the statistical errors on the GEVP results. As a consistency

![Image](054509-3)
check, we have also employed a global fit of the form of Eqs. (10) and (11) to our data. The values of $E_m$ obtained from the fit are compatible with the plateau values, and generally exhibit smaller statistical errors. We therefore consider our errors to be estimated conservatively.

### C. Computing masses

We start by recalling the definition of the $B_q$-meson mass as it has been used to nonperturbatively fix the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15]. On the lattice one combines the HQET parameters for the static quark discretizations HYP1 and HYP2 in [15].

The strange-light mass $m_{Bs} - m_{B_s}$ at the static and $O(1/m_b)$ level, reads,

$$\Delta_{s-d} m(m_s, a) = \Delta_{s-d} m(m_s, a) = \Delta_{s-d} E_{s}^{stat} + \omega_{spin} \Delta_{s-d} m + \omega_{spin} \Delta_{s-d} E_{s}^{spin},$$

respectively, where we have defined the shorthand $\Delta_{s-d} Q = Q_{m_s = m_d} - Q_{m_s = m_d}$. Finally, the mass gaps for excited states, $m_{B_q'} - m_{B_q}$, can be computed from $\Delta E_{m,n} = E_m - E_n$ via

$$\Delta_{s-d} m(m_s, a) = \Delta E_{s-d}^{stat} |_{m_q},$$

$$\Delta_{s-d} m(m_s, a) = \Delta E_{s-d}^{spin} |_{m_q},$$

Table II. Measurement details for observables in the light- and strange-quark sector. For each ensemble we list the light- and strange-quark hopping parameter, the trajectory length $\tau$, the distance of saved configurations $\tau_{cfg}$ and the exponential autocorrelation time $\tau_{exp}$ in MDU. For each individual static quark discretization we then specify the parameters

$$m_{B_q}(m_s, a) = m_{bare} + E_{s}^{stat} |_{m_q},$$

$$m_{B_q}(m_s, a) = m_{bare} + E_{s}^{stat} |_{m_q} + \omega_{kin} E_{s}^{kin} |_{m_q} + \omega_{spin} E_{s}^{spin} |_{m_q},$$

$\Delta_{q} m_{H}(m_s, a) = -\frac{4}{3} \omega_{spin} E_{s}^{spin} |_{m_q}, \quad q = s, d.$

and depends on the HQET parameter $\omega_{spin}$ and the large-volume measurement of $E_{s}^{spin}$. The strange-light mass difference $m_{B_q} - m_{B_q'}$, at the static and $O(1/m_b)$ level, reads,

$$\Delta_{s-d} m(m_s, a) = \Delta_{s-d} E_{s}^{stat} + \omega_{spin} \Delta_{s-d} m + \omega_{spin} \Delta_{s-d} E_{s}^{spin},$$

$$\Delta_{s-d} m(m_s, a) = \Delta E_{s-d}^{stat} |_{m_q},$$

$$\Delta_{s-d} m(m_s, a) = \Delta E_{s-d}^{spin} |_{m_q},$$

$\omega_{kin} E_{s}^{kin} |_{m_q}$, respectively. As any observable computed on the lattice, these quantities depend on the input parameters used in the simulation. The strange and bottom quark mass have been fixed to their physical value along the lines reported in [15, 41, 42], such that only the dependences on the light quark mass—here parameterized by $m_{Bs}$—and lattice spacing $a$ remain.

We have extracted the energies on a subset of gauge ensembles from the coordinated lattice simulations (CLS) effort for $N_t = 2$. The parameters of the simulations and the statistics entering our analysis are collected in Table I of [15]. Remaining details of the measurements have been summarized in Table II [43]. The light quark is treated in a

$$E_{s}^{stat} |_{m_q},$$

$$E_{s}^{spin} |_{m_q},$$

$\Delta_{s-d} m(m_s, a) = \Delta E_{s-d}^{stat} |_{m_q},$$

$$\Delta_{s-d} m(m_s, a) = \Delta E_{s-d}^{spin} |_{m_q},$$

$\omega_{spin} \Delta_{s-d} m + \omega_{spin} \Delta_{s-d} E_{s}^{spin},$$

$\omega_{spin} \Delta_{s-d} m + \omega_{spin} \Delta_{s-d} E_{s}^{spin},$

$\omega_{kin} E_{s}^{kin} |_{m_q},$
unitary setup with $m_\pi$ in the range $[190 \text{ MeV}, 440 \text{ MeV}]$, and the bare strange quark mass has been tuned on each CLS ensemble to its physical value by using the kaon decay constant $f_K$ to set the scale \cite{32} and $m_\pi = 494.2 \text{ MeV}$. The lattice spacings are $a/\text{fm} \in \{0.048, 0.065, 0.075\}$ for $\beta \in \{5.5, 5.3, 5.2\}$, corresponding to the CLS ensemble ids N–O, E–G, and A–B, respectively. All lattices have $m_\pi L \geq 4$, such that finite-volume effects are sufficiently exponentially suppressed at the level of accuracy we are working at.

Our data analysis takes into account correlations between different observables as well as intrinsic autocorrelations of the hybrid Monte Carlo (HMC) algorithm resulting from slow modes in the simulation. As these contributions rapidly grow towards the continuum limit, it is mandatory to estimate and include a priori unknown long-tail contributions from the autocorrelation function of each individual observable. Further details of our analysis method can be found in Appendix A.

D. Extrapolation to the physical point

To extrapolate our data to the continuum limit and to the physical point, we take expressions from heavy meson chiral perturbation theory (HM\(_\chi\)PT) if available, and a linear ansatz otherwise.

In the chiral regime, the mass of the B-meson can be extrapolated to the physical point using a functional form motivated by HM\(_\chi\)PT \cite{44}. Defining a subtracted mass by removing the leading nonanalytic (in the quark mass) term, viz.

$$m_{Bq,\delta}^{\text{sub}}(y,a) = m_B(m_\pi, a) + c_q \frac{3\hat{g}^2}{16\pi} \left( \frac{m_\pi^4}{f_K^2} \right) \frac{m_\pi^{(y/a)^3}}{(f_K^{(y/a)})^2}, \tag{17}$$

with $c_q = 1$ in HM\(_\chi\)PT at NLO for $q = d$ but zero otherwise, the parametrization reads

$$m_{Bq,\delta}^{\text{sub}}(y,a) = B_q + C_q(y - y^{\exp}) + D_q a^2. \tag{18}$$

In (17) the $B^*\to B\pi$-coupling $\hat{g} = 0.492(29)$ is taken from \cite{45} and $y = m_\pi^2/(8\pi^2 f_K^2)$ (with the convention $f_K^{\exp} = 130.4 \text{ MeV}$ and $m_\pi^{\exp} = 134.98 \text{ MeV}$). We use the same set of measurements for $f_K$ and $m_B$ on each CLS ensemble as reported in foregoing analyses \cite{15,41}. We add the subscript $\delta$ to distinguish the two available static discretizations which are combined in the extrapolation to obtain the parameter $B_q = m_{Bq}$ at the physical point $(y,a) = (y^{\exp},0)$. For the $B^*_q$-meson mass an extrapolation quadratically in the lattice spacing is justified as we have full O($a$) improvement at work in (13) at the static order and O($a^2$) terms are then suppressed by a factor $1/m_B$ once NLO terms in HQET are taken into account. For the case of $m_B$ that has been explicitly checked in \cite{15}, it is therefore conceivably valid also here for $m_{Bq}$.

In Fig. 2 we show the continuum and chiral extrapolations of $m_{Bd}$ and $m_{Bq} - m_{Bd}$ at next-to-leading order in $1/m_B$. In this and the following figures, filled symbols and dashed curves represent our HYP1 data set, while open symbols and dash-dotted curves represent our HYP2 data set. For both, equal colors and symbols refer to the same lattice spacing as indicated by equal values of the bare coupling constant $g_B^2$ in the legend; cf. Tables I and II. The solid black line is the continuum limit for the given fit ansatz.

![FIG. 2 (color online). Chiral and continuum extrapolation of $m_{Bd}$ (left) and $m_{Bq} - m_{Bd}$ (right) according to (18). The open triangle represents the corresponding result for extrapolating the static order data. Here and in the following figures, filled symbols and dashed curves represent our HYP1 data set, while open symbols and dash-dotted curves represent our HYP2 data set. The solid black line is the continuum limit for the given fit ansatz.](054509-5)
with the continuum part coinciding, in the case \( q = d \), with the expression derived in [46]. Hence, we can probe two ansätze for the chiral extrapolation by setting \( \tilde{c}_q = 0, 1 \). Since in principle the \( O(a) \) improvement of the hyperfine splitting is not implemented, we have included linear cutoff effects, but also study the scaling behavior with an \( O(a^2) \) ansatz by setting either \( \tilde{D}_{q,d} \) or \( \tilde{D}_{q,\delta} \) to zero in the equation above. In general, our data is not sensitive enough to clearly separate \( O(a) \) scaling from \( O(a^2) \) such that individual fits lead to similar results. As an additional safety measure, we account for a systematic error by increasing the uncertainty lead to similar results. As an additional safety measure, we lead to similar results. As an additional safety measure, we take the continuum limit of the leading (static) and minization. It furthermore serves as a nontrivial check that the whole procedure has been applied correctly and consistently.

### III. RESULTS

Using the HQET parameters of Table I at \( z_h = 13.25 \), we obtain for the B-meson mass \( m_B = 5.285(62) \) GeV by employing Eqs. (17) and (18) with \( c_q = 1 \) as the extrapolation ansatz. Note, however, that the experimental value \( m_B = 5.2795 \) GeV has been used as input in [15] to fix the \( b \)-quark mass. Therefore \( m_B \) is not a prediction of the theory in our setup, and the number above should be regarded as a consistency check of the approach.

#### A. Ground states

As first quantities beyond \( m_B \), we compute the \( B_s \)-meson mass and the mass difference \( m_{B_s} - m_B \). Their continuum and chiral extrapolations at next-to-leading order in \( 1/m_b \) are shown in Fig. 2 and compared to the extrapolated value of the static data at the physical point. The raw data for the mass difference \( m_{B_s} - m_B \) and the hyperfine splittings is collected in Tables III and IV.

From the extrapolation of the form of Eqs. (17) and (18) with \( c_q = 0 \), we obtain the result,
TABLE III. Mass splitting between $B_s$- and $B_d$-meson at static and next-to-leading order HQET.

<table>
<thead>
<tr>
<th>e-id</th>
<th>$y$</th>
<th>$\Delta_{s\rightarrow d}m$ [MeV]</th>
<th>$\Delta_{s\rightarrow d}m^\text{stat}$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>HYP1</td>
<td>HYP2</td>
</tr>
<tr>
<td>A4</td>
<td>0.0771(14)</td>
<td>55.2(2.6)</td>
<td>56.0(2.3)</td>
</tr>
<tr>
<td>A5</td>
<td>0.0624(13)</td>
<td>68.8(1.8)</td>
<td>66.0(1.6)</td>
</tr>
<tr>
<td>B6</td>
<td>0.0484(9)</td>
<td>71.6(4.9)</td>
<td>70.2(3.5)</td>
</tr>
<tr>
<td>E5</td>
<td>0.0926(15)</td>
<td>52.8(2.7)</td>
<td>51.9(1.9)</td>
</tr>
<tr>
<td>F6</td>
<td>0.0562(9)</td>
<td>70.9(5.7)</td>
<td>70.3(4.0)</td>
</tr>
<tr>
<td>F7</td>
<td>0.0449(8)</td>
<td>69.7(3.2)</td>
<td>74.0(2.5)</td>
</tr>
<tr>
<td>N6</td>
<td>0.0662(10)</td>
<td>64.0(6.7)</td>
<td>68.0(3.7)</td>
</tr>
<tr>
<td>O7</td>
<td></td>
<td>72.2(6.9)</td>
<td></td>
</tr>
<tr>
<td>LO-$a^2$</td>
<td>$y_{\text{exp}, a = 0}$</td>
<td>91.2(5.8)</td>
<td>87.2(5.2)</td>
</tr>
<tr>
<td>NLO-$a^2$</td>
<td>$y_{\text{exp}, a = 0}$</td>
<td>88.9(5.7)</td>
<td>85.0(5.1)</td>
</tr>
</tbody>
</table>

TABLE IV. Hyperfine splittings in the light- and strange-quark sector.

<table>
<thead>
<tr>
<th>e-id</th>
<th>$y$</th>
<th>$\Delta_{s\rightarrow d}m$ [MeV]</th>
<th>$\Delta_{s\rightarrow d}m^\text{stat}$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>HYP1</td>
<td>HYP2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HYP1</td>
<td>HYP2</td>
</tr>
<tr>
<td>A4</td>
<td>0.0771(14)</td>
<td>52.3(2.1)</td>
<td>62.0(2.4)</td>
</tr>
<tr>
<td>A5</td>
<td>0.0624(13)</td>
<td>51.1(2.0)</td>
<td>60.5(2.4)</td>
</tr>
<tr>
<td>B6</td>
<td>0.0484(9)</td>
<td>50.1(2.2)</td>
<td>58.7(2.5)</td>
</tr>
<tr>
<td>E5</td>
<td>0.0926(15)</td>
<td>51.9(2.1)</td>
<td>59.6(2.4)</td>
</tr>
<tr>
<td>F6</td>
<td>0.0562(9)</td>
<td>50.0(2.5)</td>
<td>58.1(2.7)</td>
</tr>
<tr>
<td>F7</td>
<td>0.0449(8)</td>
<td>46.1(1.9)</td>
<td>54.1(2.2)</td>
</tr>
<tr>
<td>G8</td>
<td>0.0260(5)</td>
<td>48.1(2.9)</td>
<td>53.7(2.6)</td>
</tr>
<tr>
<td>N5</td>
<td>0.0940(19)</td>
<td>52.6(2.8)</td>
<td>57.7(3.6)</td>
</tr>
<tr>
<td>N6</td>
<td>0.0662(10)</td>
<td>51.1(3.0)</td>
<td>53.3(2.9)</td>
</tr>
<tr>
<td>O7</td>
<td>0.0447(7)</td>
<td>51.7(3.7)</td>
<td>54.4(3.1)</td>
</tr>
<tr>
<td>LO-$a^2$</td>
<td>$y_{\text{exp}, a = 0}$</td>
<td>45.2(2.9)</td>
<td>43.6(2.4)</td>
</tr>
<tr>
<td>NLO-$a^2$</td>
<td>$y_{\text{exp}, a = 0}$</td>
<td>42.0(4.2)</td>
<td>37.8(3.3)</td>
</tr>
</tbody>
</table>

$m_{B_s} = 5383(63)\text{ MeV}, \quad m_{B_s} - m_{B_s}^\text{stat} = 58(12)\text{ MeV}, \quad (23)$

where the error includes statistical and systematic uncertainties (scale setting, HQET parameters), combined in quadrature as explained in Appendix A. Although our result for $m_{B_s}$ comes with a much larger error compared to the PDG value, $m_{B_s} = 5366.77 \pm 0.24 \text{ MeV}$, the difference between the mean values is only one-fourth of our error.

In the combination $m_{B_s} - m_{B_s}$, the error is reduced due to correlations among the heavy-light and heavy-strange measurements, although the latter have been performed on a subset of the available ensembles only, as it can be inferred from Table II.

Our results for the $B_s$-$B$ mass splitting at $O(1/m)$ and in the static approximation are

$$m_{B_s} - m_B = 88.9(5.7)(2.3)\chi_c \text{ MeV}, \quad (24a)$$

$$[m_{B_s} - m_B]^\text{stat} = 85.0(5.1)(2.2)\chi_c \text{ MeV}, \quad (24b)$$

both in good agreement with the PDG value of $[1]$ $m_{B_s} - m_B = 87.35(23)\text{ MeV}$. Here, the quoted mean and statistical error results from an HMxPT extrapolation ansatz that is obtained by appropriately combining Eq. (18) for the light and strange quark sector. As systematic error due to the chiral extrapolation ansatz we quote its difference to the standard $m_{B_s}^2$ extrapolation.

For the hyperfine spin splittings, we obtain

$$m_{B^*} - m_{B_s} = 41.7(4.2)(3.2)\chi_{\bar{c}}(0.3)\chi_c \text{ MeV}, \quad (25a)$$

$$m_{B^*} - m_{B_s} = 37.8(3.3)(5.8)\chi_{\bar{c}} \text{ MeV}, \quad (25b)$$

where we quote the mean value obtained with $\bar{c}_d = 1$ for the $B$-meson case and add the difference with respect to the result obtained from the ansatz with $\bar{c}_d = 0$ as a systematic error estimate for the chiral extrapolation. As mentioned earlier, we also account here for a systematic error between linear and quadratic continuum extrapolations. The $O(a)$ extrapolations are shown for both the $B$ and the $B_s$ system in Fig. 3. The filled/empty symbols at the physical point are the results using either an $O(a)$ or an $O(a^2)$ term in the continuum extrapolation.
Our result for the hyperfine splitting for the B-system is in good agreement with the experimental value \( m_{B^*} - m_B = 45.78(35) \) MeV [1], whereas the Bs hyperfine splitting differs noticeably from the experimental value \( m_{B_s^*} - m_{B_s} = 48.7^{+2.3}_{-2.1} \) MeV. Our results are smaller than the experimental value and than our result for the hyperfine splitting of the B (the opposite of the situation for the experimental values). Since the hyperfine splitting came out far too small in the quenched approximation [39], this is suggestive of a residual quenching effect from the quenching of the strange quark in our \( N_f = 2 \) simulations. Moreover, Fig. 3 indicates larger cutoff effects in the case of the hyperfine splitting for the Bs.

### B. Excited states

For the mass splittings between the ground state \( B_q \) and the first excited state, denoted here by \( B^* \) and \( B^*_q \), we obtain

\[
m_{B^*} - m_B = 791(73) \text{ MeV},
\]

\[
[m_{B^*} - m_B]^{\text{stat}} = 701(65) \text{ MeV}.
\]

after adding the individually extrapolated results for \( [m_{B^*} - m_{B^*_q}]^{\text{stat}} \) and \( [m_{B^*_q} - m_{B^*_q}]^{1/m} \). In Fig. 4 these values are shown (as pentagons, slightly shifted at the physical point) for comparison with an extrapolation according to Eq. (21). The raw data is collected in Tables V, VI, and VII.

We conclude this section by remarking that for the excited states the interpretation of our results in terms of mass differences of physical one-meson states, e.g. "radial excitations," is not straightforward. Although our values for these mass gaps are larger than what a multihadron state made of, e.g., a \( B^{(+)} \)-meson and a small number (\( \leq 2 \)) of physical pions would produce, we cannot unambiguously conclude that our \( B^*_q \) states actually correspond to radial excitations of the ground-state \( B_q \)-mesons. In a rigorous approach, states above multihadron thresholds need to be treated as resonances in order to obtain precise values for

\[
m_{B^*} - m_B = 566(57) \text{ MeV},
\]

\[
[m_{B^*} - m_{B^*_q}]^{\text{stat}} = 547(34) \text{ MeV}.
\]
their masses and widths, and to associate them with the states observable in experiments.

Since our lattice study is unquenched, the excited states can also be multiparticle states involving additional pions, beside the desired one-particle state. While it has been argued that the overlap of single-hadron interpolating operators to multihadron states is small [47,48], the two-hadron states may have a weaker volume suppression [49].

![Graph](image-url)

FIG. 5 (color online). The measured gap $m_{B_q^*} - m_{B_q}$ vs $2m_\pi$ for the excited states $B_q^*$ with $q = d$ (left) and $q = s$ (right) on each individual CLS ensemble and with HYP2 discretization of the static quark. The boxes are an estimate of the expected gap for a two-hadron state $B_q^*(-p) + \pi(p)$ with one unit of lattice momentum $p = |p| = 2\pi/L$. The lower edge of the boxes corresponds to $\Delta_q^{\text{HF}}m + \sqrt{m_q^2 + (2\pi/L)^2}$ and the upper edge includes an additional contribution $p^2/(2m_{B_q^*})$ as a naive estimate for the kinetic energy of the $B_q^*$. The dotted line is $\Delta = 2m_\pi$ corresponding to a three-hadron state $B_q + \pi + \pi$. 

### TABLE VI. Mass gaps between the excited state $B_q^*$ and the $B_q$-meson at static and next-to-leading order HQET.

<table>
<thead>
<tr>
<th>e-id</th>
<th>$y$</th>
<th>HYP1</th>
<th>HYP2</th>
<th>HYP1</th>
<th>HYP2</th>
</tr>
</thead>
<tbody>
<tr>
<td>A4</td>
<td>0.0771(14)</td>
<td>0.774(45)</td>
<td>0.748(34)</td>
<td>0.640(23)</td>
<td>0.650(22)</td>
</tr>
<tr>
<td>A5</td>
<td>0.0624(13)</td>
<td>0.760(15)</td>
<td>0.753(15)</td>
<td>0.670(11)</td>
<td>0.677(11)</td>
</tr>
<tr>
<td>B6</td>
<td>0.0484(9)</td>
<td>0.719(49)</td>
<td>0.704(35)</td>
<td>0.641(22)</td>
<td>0.641(21)</td>
</tr>
<tr>
<td>E5</td>
<td>0.0926(15)</td>
<td>0.791(66)</td>
<td>0.676(44)</td>
<td>0.609(29)</td>
<td>0.624(25)</td>
</tr>
<tr>
<td>F6</td>
<td>0.0562(9)</td>
<td>0.689(30)</td>
<td>0.722(24)</td>
<td>0.643(18)</td>
<td>0.642(17)</td>
</tr>
<tr>
<td>F7</td>
<td>0.0449(8)</td>
<td>0.665(24)</td>
<td>0.660(19)</td>
<td>0.593(15)</td>
<td>0.601(14)</td>
</tr>
<tr>
<td>N6</td>
<td>0.0662(10)</td>
<td>0.698(49)</td>
<td>0.718(36)</td>
<td>0.621(38)</td>
<td>0.643(32)</td>
</tr>
<tr>
<td>O7</td>
<td>0.0447(7)</td>
<td>0.736(38)</td>
<td></td>
<td>0.669(29)</td>
<td></td>
</tr>
<tr>
<td>LO-$a^2$</td>
<td>$y^{\text{exp}}, a = 0$</td>
<td>0.570(47)</td>
<td></td>
<td>0.547(34)</td>
<td></td>
</tr>
<tr>
<td>LO-$a^1$</td>
<td>$y^{\text{exp}}, a = 0$</td>
<td>0.519(74)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### TABLE VII. Subleading HQET contributions to the mass gaps between excited and ground states.

<table>
<thead>
<tr>
<th>e-id</th>
<th>$y$</th>
<th>HYP1</th>
<th>HYP2</th>
<th>HYP1</th>
<th>HYP2</th>
</tr>
</thead>
<tbody>
<tr>
<td>A4</td>
<td>0.0771(14)</td>
<td>73(27)</td>
<td>78(21)</td>
<td>133(38)</td>
<td>98(26)</td>
</tr>
<tr>
<td>A5</td>
<td>0.0624(13)</td>
<td>71(11)</td>
<td>75(8)</td>
<td>90(11)</td>
<td>76(9)</td>
</tr>
<tr>
<td>B6</td>
<td>0.0484(9)</td>
<td>70(31)</td>
<td>73(20)</td>
<td>78(45)</td>
<td>64(28)</td>
</tr>
<tr>
<td>E5</td>
<td>0.0926(15)</td>
<td>77(17)</td>
<td>75(9)</td>
<td>182(71)</td>
<td>52(40)</td>
</tr>
<tr>
<td>F6</td>
<td>0.0562(9)</td>
<td>61(31)</td>
<td>68(21)</td>
<td>47(24)</td>
<td>80(17)</td>
</tr>
<tr>
<td>F7</td>
<td>0.0449(8)</td>
<td>82(18)</td>
<td>80(11)</td>
<td>71(19)</td>
<td>59(15)</td>
</tr>
<tr>
<td>G8</td>
<td>0.0260(5)</td>
<td>36(26)</td>
<td>54(15)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N5</td>
<td>0.0940(19)</td>
<td>132(110)</td>
<td>6(95)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N6</td>
<td>0.0662(10)</td>
<td>149(59)</td>
<td>94(31)</td>
<td>77(31)</td>
<td>76(18)</td>
</tr>
<tr>
<td>O7</td>
<td>0.0447(7)</td>
<td>75(25)</td>
<td>84(17)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LO-$a^1$</td>
<td>$y^{\text{exp}}, a = 0$</td>
<td>0.090(40)</td>
<td></td>
<td>0.019(46)</td>
<td></td>
</tr>
</tbody>
</table>
Moreover, a chiral extrapolation linear in $m_q^2$ might not be adequate for a multihadron state, and a different extrapolation ansatz for these states, e.g., linear in $m_q$, might also yield somewhat smaller mass gaps.

In continuum (and infinite-volume) physics, any excited $B_q$-meson state, $B_q^*$, which strongly decays into an $\ell$-wave $B_q + \pi$ state, i.e., a resonance in the $\ell$-wave $B_q + \pi$ scattering channel, implies that the corresponding two-hadron state $B_q^* + \pi$ with relative angular momentum $\ell$ has the correct quantum numbers to couple to our interpolating operators used for the $B_q$. For the $q = d$ sector, the set of possible two-hadron excited states includes

(i) $B^* + \pi$ in P-wave which would have a noninteracting two-hadron energy gap of $\Delta \gtrsim 181$ MeV,

(ii) $B^{*0} + \pi$ in P-wave, where $B^{*0}$ is a radial excitation ($J^P = 1^-$),

(iii) $B_0^* + \pi$ in S-wave, where $B_0^*$ is an orbital excitation ($J^P = 0^+$),

(iv) $B_2^* + \pi$ in D-wave, where $B_2^*$ is an orbital excitation ($J^P = 2^+$), like the observed $B_2^*(5747)^0$ state which would lead to a noninteracting two-hadron energy gap of $\Delta \gtrsim 598$ MeV.

On a finite lattice, the energies of states with nonzero relative angular momentum are lifted due to the minimal volume energy spectrum of the excited state we observe.

In Figs. 5 and 6 we show our data points on the various two-hadron states. The comparison indicates that some of the two-hadron states can be close in energy to the excited states we measured. Depending on the pion mass on a given ensemble, the energy gaps determined according to Eqs. (16) may in fact be the energy splitting to the lowest lying $B^* + \pi$ state, if this is lighter than the radial excitations $B_q^*$.

Below three- or more-hadron thresholds, the infinite volume scattering matrix (up to corrections which vanish exponentially in the spatial lattice extent) may be inferred from the finite volume energy spectrum [50–54]. In practice this requires the construction of correlation matrices containing two-hadron as well as single-hadron operators. To date, this procedure has been carried out successfully in some simple systems such as $\pi - \pi$ and $\pi - K$ scattering, and the energy dependence of the scattering phase shift has been determined with sufficient resolution to clearly discern resonant behavior (see e.g., [55] for a recent review). Without performing such a dedicated study, we are not able to conclusively determine the nature of the excited state we observe.

IV. CONCLUSIONS

In this paper, we have presented results for the B-meson spectrum obtained in the framework of lattice HQET expanded to $O(1/m_b)$. Within this approach the existence of a continuum limit is guaranteed, as numerically tested with high accuracy in previous studies [56, 57]. In contrast to the HQET expansion in continuum perturbation theory, our approach is manifestly nonperturbative in the strong coupling. We perform the continuum extrapolation from lattice resolutions in the range 0.08–0.05 fm. Pion masses, in our setup with $N_f = 2$ degenerate flavors, reach down to values of about 190 MeV. The accuracy is at the 10% level, for the different splittings presented (e.g., hyperfine and $B_d$–$B_s$ splittings), and we always find consistency within 2 standard deviations with values from the PDG, whenever a comparison is possible.

Hyperfine splittings probe higher-order terms in HQET and the reported results represent an important check on the validity and the reliability of the asymptotic HQET expansion, truncated at NLO, at the b-quark mass scale. Compared to previous quenched results, we observe a significant shift for the hyperfine splitting in the B-meson sector, which now agrees with the experimental determination. In our $N_f = 2$ simulations, the hyperfine splitting in the $B_s$ sector appears to suffer from a residual quenching effect, which is in line with what was seen for $N_f = 0$. In order to ascertain that the quenching of the strange quark is indeed the root cause of the reduced $B_s$ hyperfine splitting seen here, we plan to extend our computations to simulations of the $N_f = 2 + 1$ theory [58].

A dominant source of uncertainty in our results is represented by cutoff effects (see Table VIII). This is not unexpected since we have not implemented $O(a)$ improvement at $O(1/m_b)$. While implementing a fully nonperturbative improvement program at this order is probably too difficult, one may consider perturbative (tree-level or one-loop) improvement for future applications.
Knowledge of the mass splittings is relevant for the computation of hadronic parameters within the sum-rules approach and when comparing results from the lattice to sum-rules estimates. The mass gaps of excited states are

We also determined the mass gaps for excited states in both the B and the $B_s$ sectors. The results are consistent with a radial splitting, e.g. as computed for the $B_s$ system in [9], but these excited states might also be two- or multihadron states.

<table>
<thead>
<tr>
<th>Source</th>
<th>$m_{B_s}$</th>
<th>$m_{B_s} - m_B$</th>
<th>$m_{B_s^*} - m_{B_s}$</th>
<th>$m_{B_s} - m_B$</th>
<th>$m_{B_s^*} - m_B$</th>
<th>$m_{B_s} - m_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A4</td>
<td>0.46%</td>
<td>2.52%</td>
<td>3.51%</td>
<td>12.48%</td>
<td>9.79%</td>
<td>9.93%</td>
</tr>
<tr>
<td>A5</td>
<td>0.30%</td>
<td>1.32%</td>
<td>1.81%</td>
<td>3.14%</td>
<td>6.67%</td>
<td>5.78%</td>
</tr>
<tr>
<td>B6</td>
<td>0.03%</td>
<td>1.50%</td>
<td>0.39%</td>
<td>0.23%</td>
<td>1.04%</td>
<td>0.06%</td>
</tr>
<tr>
<td>E5</td>
<td>0.28%</td>
<td>0.40%</td>
<td>1.80%</td>
<td>0.46%</td>
<td>4.72%</td>
<td>1.51%</td>
</tr>
<tr>
<td>F6</td>
<td>0.10%</td>
<td>0.34%</td>
<td>0.45%</td>
<td>8.62%</td>
<td>5.07%</td>
<td>6.72%</td>
</tr>
<tr>
<td>F7</td>
<td>0.21%</td>
<td>0.82%</td>
<td>1.50%</td>
<td>34.56%</td>
<td>17.87%</td>
<td>23.42%</td>
</tr>
<tr>
<td>G8</td>
<td>0.53%</td>
<td>5.25%</td>
<td>0.00%</td>
<td>0.05%</td>
<td>6.46%</td>
<td>0.03%</td>
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<tr>
<td>N5</td>
<td>1.90%</td>
<td>8.04%</td>
<td>0.45%</td>
<td>0.01%</td>
<td>7.94%</td>
<td>0.05%</td>
</tr>
<tr>
<td>N6</td>
<td>5.97%</td>
<td>1.33%</td>
<td>29.18%</td>
<td>31.56%</td>
<td>14.60%</td>
<td>27.70%</td>
</tr>
<tr>
<td>O7</td>
<td>4.50%</td>
<td>6.34%</td>
<td>13.49%</td>
<td>8.05%</td>
<td>25.32%</td>
<td>14.42%</td>
</tr>
</tbody>
</table>

We also determined the mass gaps for excited states in both the B and the $B_s$ sectors. The results are consistent with a radial splitting, e.g. as computed for the $B_s$ system in [9], but these excited states might also be two- or multihadron states.

Knowledge of the mass splittings is relevant for the computation of hadronic parameters within the sum-rules approach and when comparing results from the lattice to sum-rules estimates. The mass gaps of excited states are
also important information for the computation of form factors on the lattice, for example for the $B \rightarrow \pi \ell^\nu$ and the $B_s \rightarrow K \ell^\nu$ decays, as currently endeavored by the ALPHA Collaboration [12,14], and in general in the spectral analysis of two- and three-point functions.

ACKNOWLEDGMENTS

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APPENDIX A: DETERMINATION OF THE STATISTICAL ERROR IN THE PRESENCE OF AUTOCORRELATIONS

In order to compute the statistical error in the presence of both correlations between the different observables and of autocorrelations along the HMC trajectories by which our ensembles were generated, we employ the methods of [59–62], which we briefly outline below.

The starting point is the computation of the “primary” observables $C^i_{\alpha}$, where $i$ labels the $N_{\text{meas}}$ gauge configurations, and $\alpha$ is an aggregate label for the different correlators measured (stat, spin, kin), the Euclidean time separation $\tau$ between the source and sink, and the different

\begin{table}
\centering
\caption{Raw data for plateau-averaged ground state energies in the heavy-strange sector. The subscript to the statistical error is the value of $t_{\text{min}}$ in the GEVP analysis.}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
$e$-id & HYP1 & $aE_{n=1}^{\text{stat}}$ & HYP2 & $aE_{n=1}^{\text{stat}}$ & HYP1 & $a^2E_{n=1}^{\text{kin}}$ & HYP2 & $a^2E_{n=1}^{\text{kin}}$ & HYP1 & $-a^2E_{n=1}^{\text{spin}}$ & HYP2 & $-a^2E_{n=1}^{\text{spin}}$
\hline
A4 & 0.43905(46) & 0.04030(40) & 0.8585(7) & 0.9024(5) & 0.02365(22) & 0.02220(17) &
A5c & 0.43856(53) & 0.04037(46) & 0.8590(11) & 0.9006(7) & 0.02308(29) & 0.02214(24) &
B6 & 0.43224(41) & 0.39722(32) & 0.8556(4) & 0.8990(3) & 0.02273(11) & 0.02139(9) &
E5 & 0.40063(44) & 0.36736(36) & 0.8157(11) & 0.8567(9) & 0.01820(31) & 0.01753(21) &
F6 & 0.39468(35) & 0.36063(27) & 0.8122(6) & 0.8530(4) & 0.01683(12) & 0.01612(9) &
F7 & 0.39217(66) & 0.35837(54) & 0.8118(11) & 0.8534(7) & 0.01627(22) & 0.01576(16) &
N6 & 0.32827(44) & 0.29799(33) & 0.7429(11) & 0.7758(6) & 0.00991(18) & 0.00941(12) &
O7 & $\cdots$ & 0.29571(34) & 0.7753(8) & & & &
\hline
\end{tabular}
\end{table}

\begin{table}
\centering
\caption{Raw data for plateau-averaged 1st excited state energies in the heavy-strange sector. The subscript to the statistical error is the value of $t_{\text{min}}$ in the GEVP analysis.}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
$e$-id & HYP1 & $aE_{n=2}^{\text{stat}}$ & HYP2 & $aE_{n=2}^{\text{stat}}$ & HYP1 & $a^2E_{n=2}^{\text{kin}}$ & HYP2 & $a^2E_{n=2}^{\text{kin}}$ & HYP1 & $-a^2E_{n=2}^{\text{spin}}$ & HYP2 & $-a^2E_{n=2}^{\text{spin}}$
\hline
A4 & 0.6829(77) & 0.6519(69) & 0.995(35) & 0.999(23) & 0.0250(12) & 0.0217(10) &
A5c & 0.6936(63) & 0.6614(58) & 0.952(20) & 0.975(15) & 0.0243(16) & 0.0212(13) &
B6 & 0.6762(61) & 0.6411(54) & 0.934(33) & 0.960(21) & 0.0224(11) & 0.0201(9) &
E5 & 0.6022(82) & 0.5740(73) & 0.950(47) & 0.894(30) & 0.0170(17) & 0.0162(13) &
F6 & 0.6074(42) & 0.5730(37) & 0.855(13) & 0.914(8) & 0.0199(26) & 0.0147(18) &
F7 & 0.5885(68) & 0.5573(62) & 0.873(22) & 0.902(13) & 0.0186(16) & 0.0167(12) &
N6 & 0.4803(75) & 0.4554(58) & 0.781(12) & 0.813(7) & 0.0107(8) & 0.0105(6) &
O7 & 0.4594(49) & & 0.807(9) & & & &
\hline
\end{tabular}
\end{table}
smearing levels employed at source and sink. The gauge average \( \bar{C}_a \) and the variance \( \sigma_{\bar{C}_a}^2 \) are computed as usual. To estimate the true statistical error \( \sigma^{\bar{C}_a} \) of the gauge average, we also require the integrated autocorrelation time \( \tau^{\text{int}}_{\bar{C}_a} \), which is computed from the autocorrelation function

\[
\Gamma^{(1)}_{\text{int}} = \Gamma_{\bar{C}_a}C_{\bar{C}_a}(\tau) = \lim_{k\to\infty} \frac{1}{k} \sum_{i=1}^{K} (C^{\tau + i}_a - \bar{C}_a)(C^\tau_\beta - \bar{C}_\beta),
\]

(A1)

where \( \tau \) is the separation in simulation time along the Markov chain. In order to take into account the long-time tail of \( \Gamma \), the conservative estimate [60]

\[
\tau^{\text{int}}_{\bar{C}_a} = \frac{1}{2} + \frac{1}{\Gamma^{(1)}_{\text{int}}(0)} \left( \sum_{i=1}^{W-1} \Gamma^{(1)}_{\text{int}}(\tau) + \tau^{\exp} \Gamma^{(1)}_{\text{int}}(W) \right)
\]

(A2)

is used, where \( \tau^{\exp} \) is an estimate of the exponential autocorrelation time of the Markov chain. The values used in our analysis are listed in Table II. The window size \( W \) is automatically chosen as the point \( \tau = W \) where \( \Gamma^{(1)}(\tau) \) comes close to zero within about 1.5 of its estimated error. The true statistical error is then given by

\[
\sigma^{\bar{C}_a} = 2\tau^{\text{int}}_{\bar{C}_a} \sigma^{\bar{C}_a}_{\text{meas}}.
\]

For derived observables \( D_{\alpha'} \), which are functions of gauge averages of the primary observables \( \bar{C}_{\alpha'} \), and in our case include the generalized eigenvalues and eigenvectors as well as the energies derived from them, we compute the derivatives

\[
J_{\alpha'} = \frac{\partial D_{\alpha'}}{\partial \bar{C}_{\alpha}}
\]

and the autocorrelation function [60]

\[
\Gamma^{(2)}_{\alpha'\beta'}(\tau) \equiv \sum_{\alpha,\beta} J_{\alpha\beta} \Gamma^{(1)}_{\alpha \beta}(\tau) J_{\beta'\alpha'}.
\]

(A5)

The variance of the derived observable \( D_{\alpha'} \) is then given by

\[
\sigma^{2}_{D_{\alpha'}} = \Gamma^{(2)}_{\alpha'\alpha'}(0)
\]

(A6)

and its statistical error by

\[
\sigma^{2}_{D_{\alpha'}} = 2\tau^{\text{int}}_{D_{\alpha'}} \sigma^{2}_{D_{\alpha'}}_{\text{meas}},
\]

(A7)

where the integrated autocorrelation time \( \tau^{\text{int}}_{D_{\alpha'}} \) is again estimated using (A2), with \( \Gamma^{(2)} \) substituted for \( \Gamma^{(1)} \).

Since the extraction of plateau values from a weighted fit requires knowledge of the errors of the individual points, in principle this procedure should be iterated, with the plateau averages as secondary derived observables of the derived observables. However, the integrated autocorrelation times for the effective energies in the plateau region do not markedly differ. Therefore, it is sufficient to employ their variances (as estimated using e.g. a jackknife procedure for error propagation) to weight the fit, treating only the fitted values as derived observables. This simplified procedure has been adopted here.

In order to extract the final answer in physical units, the plateau values must be combined with each other and with the HQET parameters and lattice spacing, propagating the errors on each of those to the final result, where the HQET parameters are statistically independent of the large-volume observables; similarly, in extrapolating to the chiral and continuum limits, the results obtained from different ensembles are statistically independent, and their contribution to the error of the final result \( f \) can thus be added in quadrature:

\[
\sigma^{2}_{f} = \sum_{e} \sigma^{2}_{f}(e) + \sum_{i,j} \frac{\partial f}{\partial Y_i} \frac{\partial f}{\partial Y_j},
\]

(A8)

where the \( Y_i \) are the additional parameters, \( C_{\gamma,Y} \) is their (known) covariance matrix, and \( \sigma^{2}_{f}(e) \) is the error computed according to Eq. (A7) when taking into account only the fluctuations of \( \bar{C}_a \) on ensemble \( e \) [60–62].

**APPENDIX B: EFFECTIVE ENERGIES AND MATRIX ELEMENTS**

In this Appendix we provide the numerical results of our GEVP analysis after performing a weighted plateaux average

\[
E^x_n = \frac{\sum w(t) E^{\text{eff},x}(t, t_0)}{\sum w(t)}
\]

\[
w(t) = (\sigma[E^{\text{eff},x}(t, t_0)])^{-2}
\]

for \( t \in [t_{\text{min}}, t_{\text{max}}] \) and \( t_0 \geq t_{\text{min}}/2 \); see Sec. II B. The specific value of \( t_{\text{max}} \) is irrelevant due to noise dominated data at large time separations. [63] As a consequence of the exponential growth of the noise-to-signal ratio, the quoted errors are dominated by the error at \( t_{\text{min}} \) and we decided to quote \( t_{\text{min}} \) as a subscript to the statistical error in the following Tables IX–XIV. For determining \( t_{\text{min}} \), we use \( t_0 = t - 1 \) in the GEVP, and then \( t_0 = t_{\text{min}} - 1 \) once \( t_{\text{min}} \) is fixed. The errors quoted are those entering the corresponding effective energy plots (Figs. 7–17) presented below and do not contain the tail contribution of the error. Since the autocorrelation is expected to be the same among different time slices in the plateau region, it does not affect the estimate (B1) and can be added, including the exponential tail, whenever needed explicitly. In fact, all values quoted for derived observables as presented in the main text have the exponential tail included as discussed in Appendix A.

The same procedure has been used to obtain matrix elements \( p^x \). We include them in the present paper (Table XIII–XIV) in order to complete the data set used in [15,41].
TABLE XIII. Raw data for plateau-averaged ground state matrix elements in the heavy-light sector. The subscript to the statistical error is the value of $t_{\text{min}}$ in the GEVP analysis.

<table>
<thead>
<tr>
<th>e-id</th>
<th>$a^{3/2} p^{{\text{stat}}}_{n=1}$</th>
<th>HYP2</th>
<th>HYP1</th>
<th>$-a p^{{\text{kin}}}_{n=1}$</th>
<th>HYP2</th>
</tr>
</thead>
<tbody>
<tr>
<td>A4</td>
<td>0.1223(5)_{10}</td>
<td>0.1036(4)_{10}</td>
<td>1.482(37)_{3}</td>
<td>0.727(35)_{3}</td>
<td></td>
</tr>
<tr>
<td>A5c</td>
<td>0.1205(4)_{9}</td>
<td>0.1018(3)_{9}</td>
<td>1.501(19)_{3}</td>
<td>0.748(19)_{3}</td>
<td></td>
</tr>
<tr>
<td>A5d</td>
<td>0.1192(6)_{9}</td>
<td>0.1012(5)_{9}</td>
<td>1.503(26)_{3}</td>
<td>0.749(26)_{3}</td>
<td></td>
</tr>
<tr>
<td>B6</td>
<td>0.1144(13)_{11}</td>
<td>0.0970(10)_{11}</td>
<td>1.473(44)_{7}</td>
<td>0.743(41)_{7}</td>
<td></td>
</tr>
<tr>
<td>E5</td>
<td>0.0984(4)_{11}</td>
<td>0.0849(3)_{11}</td>
<td>1.360(30)_{3}</td>
<td>0.703(30)_{3}</td>
<td></td>
</tr>
<tr>
<td>F6</td>
<td>0.0918(10)_{12}</td>
<td>0.0787(8)_{12}</td>
<td>1.329(49)_{3}</td>
<td>0.668(45)_{3}</td>
<td></td>
</tr>
<tr>
<td>F7</td>
<td>0.0896(9)_{12}</td>
<td>0.0776(7)_{12}</td>
<td>1.299(52)_{3}</td>
<td>0.654(48)_{3}</td>
<td></td>
</tr>
<tr>
<td>G8</td>
<td>0.0870(13)_{11}</td>
<td>0.0755(10)_{11}</td>
<td>1.370(56)_{6}</td>
<td>0.703(52)_{7}</td>
<td></td>
</tr>
<tr>
<td>N5</td>
<td>0.0620(6)_{15}</td>
<td>0.0555(5)_{15}</td>
<td>1.126(40)_{3}</td>
<td>0.615(37)_{9}</td>
<td></td>
</tr>
<tr>
<td>N6</td>
<td>0.0580(11)_{16}</td>
<td>0.0510(7)_{16}</td>
<td>1.145(69)_{10}</td>
<td>0.599(61)_{10}</td>
<td></td>
</tr>
<tr>
<td>O7</td>
<td>0.0559(13)_{16}</td>
<td>0.0490(9)_{16}</td>
<td>1.134(62)_{3}</td>
<td>0.617(56)_{9}</td>
<td></td>
</tr>
</tbody>
</table>

TABLE XIV. Raw data for plateau-averaged ground state matrix elements in the heavy-strange sector.

<table>
<thead>
<tr>
<th>e-id</th>
<th>$a^{3/2} p^{{\text{stat}}}_{n=1}$</th>
<th>HYP2</th>
<th>HYP1</th>
<th>$-a p^{{\text{kin}}}_{n=1}$</th>
<th>HYP2</th>
</tr>
</thead>
<tbody>
<tr>
<td>A4</td>
<td>0.13448(77)_{10}</td>
<td>0.11329(58)_{10}</td>
<td>1.553(37)_{7}</td>
<td>0.757(36)_{7}</td>
<td></td>
</tr>
<tr>
<td>A5</td>
<td>0.13457(78)_{9}</td>
<td>0.11269(60)_{9}</td>
<td>1.563(34)_{6}</td>
<td>0.781(33)_{6}</td>
<td></td>
</tr>
<tr>
<td>B6</td>
<td>0.13143(50)_{11}</td>
<td>0.11041(37)_{11}</td>
<td>1.536(31)_{8}</td>
<td>0.747(29)_{8}</td>
<td></td>
</tr>
<tr>
<td>E5</td>
<td>0.10746(71)_{12}</td>
<td>0.09264(51)_{12}</td>
<td>1.391(41)_{8}</td>
<td>0.712(39)_{8}</td>
<td></td>
</tr>
<tr>
<td>F6</td>
<td>0.10521(47)_{13}</td>
<td>0.09091(34)_{13}</td>
<td>1.387(35)_{9}</td>
<td>0.689(31)_{9}</td>
<td></td>
</tr>
<tr>
<td>F7</td>
<td>0.10296(82)_{13}</td>
<td>0.08857(61)_{13}</td>
<td>1.403(38)_{8}</td>
<td>0.703(38)_{8}</td>
<td></td>
</tr>
<tr>
<td>N6</td>
<td>0.06562(56)_{16}</td>
<td>0.05788(40)_{16}</td>
<td>1.173(46)_{10}</td>
<td>0.611(41)_{10}</td>
<td></td>
</tr>
<tr>
<td>O7</td>
<td>0.05745(48)_{15}</td>
<td>0.05745(48)_{15}</td>
<td>0.620(39)_{9}</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>e-id</th>
<th>$a p^{{\text{stat}}}_{n=1}$</th>
<th>HYP2</th>
<th>HYP1</th>
<th>$a p^{{\text{spin}}}_{n=1}$</th>
<th>HYP2</th>
</tr>
</thead>
<tbody>
<tr>
<td>A4</td>
<td>0.4426(9)_{10}</td>
<td>0.39451(72)_{10}</td>
<td>0.4778(9)_{5}</td>
<td>0.4488(9)_{5}</td>
<td></td>
</tr>
<tr>
<td>A5c</td>
<td>0.4395(10)_{9}</td>
<td>0.39354(72)_{9}</td>
<td>0.4782(13)_{5}</td>
<td>0.4493(12)_{5}</td>
<td></td>
</tr>
<tr>
<td>B6</td>
<td>0.4374(8)_{12}</td>
<td>0.39070(61)_{12}</td>
<td>0.4799(5)_{3}</td>
<td>0.4505(5)_{3}</td>
<td></td>
</tr>
<tr>
<td>E5</td>
<td>0.4164(10)_{12}</td>
<td>0.36767(78)_{12}</td>
<td>0.4675(10)_{6}</td>
<td>0.4393(9)_{6}</td>
<td></td>
</tr>
<tr>
<td>F6</td>
<td>0.4117(6)_{12}</td>
<td>0.36459(42)_{12}</td>
<td>0.4658(6)_{3}</td>
<td>0.4398(5)_{3}</td>
<td></td>
</tr>
<tr>
<td>F7</td>
<td>0.4094(12)_{13}</td>
<td>0.36180(93)_{13}</td>
<td>0.4670(10)_{6}</td>
<td>0.4395(8)_{6}</td>
<td></td>
</tr>
<tr>
<td>N6</td>
<td>0.3605(13)_{16}</td>
<td>0.31679(90)_{16}</td>
<td>0.4364(10)_{8}</td>
<td>0.4165(9)_{8}</td>
<td></td>
</tr>
<tr>
<td>O7</td>
<td>0.31636(88)_{15}</td>
<td>0.31636(88)_{15}</td>
<td>0.4176(13)_{8}</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
A special case is the ensemble labeled A5 for which we have two independent Monte Carlo histories/replicas (A5c and A5d). Here, measurements and a subsequent GEVP analysis have been independently performed for both replicas in the heavy-light sector but only on A5d for heavy-strange. The results from different replicas are then combined before derived observables as presented in the main text are computed.
FIG. 8 (color online). Effective energies $E^{\text{eff}}_{n, \delta}$ following our GEVP analysis in the heavy-light (top) and heavy-strange (bottom) sector on ensemble A5c.
FIG. 9 (color online). Effective energies $E_{\eta,\delta}^{\text{eff}}$ following our GEVP analysis in the heavy-strange sector on ensemble A5d.
FIG. 10 (color online). Effective energies $E_{n,\delta}^{\text{eff}}$ following our GEVP analysis in the heavy-light (top) and heavy-strange (bottom) sector on ensemble B6.
FIG. 11 (color online). Effective energies $E^{\text{eff}}_{n,\delta}$ following our GEVP analysis in the heavy-light (top) and heavy-strange (bottom) sector on ensemble E5g.
FIG. 12 (color online). Effective energies $E_{\text{eff},n}^{\text{GEVP}}$ following our GEVP analysis in the heavy-light (top) and heavy-strange (bottom) sector on ensemble F6.
FIG. 13 (color online). Effective energies $E_{\text{eff},x}^{n,\delta}$ following GEVP analysis in the heavy-light (top) and heavy-strange (bottom) sector on ensemble F7.
FIG. 14 (color online). Effective energies $E_{\eta,\delta}^{\text{eff,x}}$ following our GEVP analysis in the heavy-light sector on ensemble G8.

FIG. 15 (color online). Effective energies $E_{\eta,\delta}^{\text{eff,x}}$ following our GEVP analysis in the heavy-light sector on ensemble N5.
FIG. 16 (color online). Effective energies $E_{\text{eff}, n, \delta}$ following our GEVP analysis in the heavy-light (top) and heavy-strange (bottom) sector on ensemble N6.
FIG. 17 (color online). Effective energies $E_{\text{eff}}^{x}$ following our GEVP analysis for heavy-light (top) and heavy-strange (bottom) sector on ensemble O7c.
[43] For the B6-ensemble a preliminary value of $\kappa_s$ has been used, which produces a bare subtracted quark mass which differs by about 1 MeV from the final one.
[63] For plotting convenience we set $t_{\text{max}} / a = \infty$ in the plots.