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Predicting the spectrum and decay constants of positive-parity heavy-strange mesons using domain-wall fermions

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We present a lattice-QCD calculation of the masses and decay constants of the positive-parity heavy-strange mesons D_{s0}^*, D_{s1}, B_{s0}^*, and B_{s1}. The calculations are performed with domain-wall fermions for the light and strange quarks and an anisotropic clover action for the charm and bottom quarks. We use seven different RBC/UKQCD ensembles with pion masses ranging from a near-physical 139 MeV up to 431 MeV. We consider two different analysis types, with or without two-meson operators at the source. We observe the expected below-threshold ground states. The fits without the two-meson operators appear to be more stable, but may overestimate the ground-state energies, while preliminary fits with two-meson operators at the source only appear to underestimate the ground-state energies.

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1. Introduction

There has been considerable interest in the positive-parity heavy-strange mesons since the 2003 discovery of the $D^*_{s0}(2317)^\pm$ by the BaBar collaboration [1, 2]. The $D^*_{s0}(2317)^\pm$ state lies ~ 45 MeV below the DK kinematic threshold, which is far away from the $n^{2s+1}\ell_J = 1^3P_0\ q\bar{q}$ state expected from potential models. For example, *Godfrey and Kokoski* predict a broad resonance above threshold [3]. This discrepancy prompts an interpretation of the $D^*_{s0}(2317)^\pm$ as an exotic state. Further possibly non-$q\bar{q}$ states are known from experiment, including the $J^P = 1^+\ D_{s1}(2460)^\pm$ sitting below and near the D^*K threshold, as shown in Table 1.

The D^*_{s0} and D_{s1} states have been identified as candidates for a molecular structure [1, 4], that is, a four-quark state consisting of two shallowly bound $q\bar{q}$ color singlet pairs. This is based on key features such as nearness to the threshold and a relatively strong coupling to the meson-meson scattering-state decay channel [5]. Weinberg's compositeness criterion is also applicable to assess the molecular structure of mesons [4, 6]. Lattice studies of the positive-parity D_s spectrum date back to 1997 [7], preceding the $D^*_{s0}(2317)^\pm$ discovery. These early studies failed to resolve the below-threshold state. After introducing interpolating fields of the form of two-meson pairs, a number of works have found a spectrum consistent with the BaBar measurements [8, 9]. Further recent results for the D^*_{s0} at heavier pion masses are reported in Refs. [10, 11].

In the bottom-strange sector, less is known about the positive-parity spectrum from experiment. The $B_{s1}(5830)$, as well as more massive states not yet assigned a spin, have been identified above threshold and are expected to be excited states. The ground states B^*_{s0} and B_{s1} have been studied on the lattice [12–14], and their proximity to the $B^{(*)}K$ thresholds also raises the possibility of molecular structures.

Another interesting feature of the heavy-strange scalar and axial vector mesons is their relationship with form factors for semileptonic decays, which may be used to probe new physics. Discrepancies between SM predictions and LHC measurements of branching fractions and angular observables have been observed for some processes involving semileptonic b decays (the so-called "b anomalies") [15]. Currents for $b \to s$ (or $c \to s$) transitions have overlap with heavy-strange two-meson scattering pairs, and the form factors inherit the pole structure of the $B^{(*)}K$ ($D^{(*)}K$) amplitudes. Precise knowledge of the pole locations is helpful in parametrizing the form factors. Furthermore, when considering unitarity bounds on the form factors, the contributions from single-particle bound states in these amplitudes depend on their decay constants (see, e.g., Ref. [16]). The decay constants are known with high precision for the ground-state negative-parity heavy-strange mesons [17], but are less well known in the positive-parity case. For the positive-parity mesons, the decay constants are defined through $\langle 0|\, J^\mu_V \left|H^*_{s0}\right\rangle = i f_{H^*_{s0}} p^\mu$ and $\langle 0|\, J^\mu_A \left|H_{s1}\right\rangle = f_{H_{s1}} m_{H_{s1}} \epsilon^\mu$, where $J^\mu_V = \bar{Q}\gamma^\mu s$ and $J^\mu_A = \bar{Q}\gamma^\mu\gamma_5 s$.

The positive-parity charm-strange decay constants $f_{D^*_{s0}}$ and $f_{D_{s1}}$ have previously been calculated on the lattice [9]. For the bottom-strange decay constants $f_{B^*_{s0}}$ and $f_{B_{s1}}$, there appear to be no published lattice calculations, but there are estimates from QCD sum rules and other methods (see, e.g., Refs. [18, 19]). In the following, we present preliminary results from a new lattice-QCD study of the positive-parity heavy-strange mesons, including, for the first time, the decay constants of the B^*_{s0} and B_{s1}.

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$n^{2s+1}\ell_J$	J^P	State	Mass
1^1S_0	0^-	$D_s^\pm$	1968 MeV
1^3S_1	1^-	$D_s^{*\pm}$	2112 MeV
1^3P_0	0^+	$D_{s0}^*(2317)^\pm$	2318 MeV
1^3P_1	1^+	$D_{s1}(2460)^\pm$	2460 MeV
1^1P_1	1^+	$D_{s1}(2536)^\pm$	2535 MeV

Table 1: Observed D_s states [20]. The DK and D^*K kinematic thresholds are located at $\sim$ 2.36 GeV and $\sim$ 2.50 GeV, respectively.

2. Lattice Action and Ensemble Details

Our simulations use Iwasaki-action gauge configurations with 2+1 dynamical domain-wall fermions produced by the RBC/UKQCD collaboration [21, 22]. Domain-wall fermions allow for exact chiral symmetry at finite lattice spacing where 4D chiral fermions are realized as low-energy degrees of freedom from a structure in a 5th dimension [23]. Of the 7 ensembles on which simulations are run (Table 2), C00078 and F1M use the Möbius domain-wall fermion formulation of *Brower, Neff and Orginos* [24], and the others use the formulation of *Shamir* [25].

Table 2 contains the lattice spacings, sizes, light and (partially quenched) strange-quark masses for each of our ensembles (see also [26]). Correlation functions are constructed via covariant approximation averaging [27] over different source locations, using a total of $N_{\rm ex}$ and $N_{\rm sl}$ "exact" and "sloppy" samples on each ensemble. The sloppy samples were obtained using propagators with reduced conjugate-gradient iteration count, combined with low-mode deflation for the light quarks.

Ensemble C00078 has a near-physical pion mass, and all ensembles have large volumes, corresponding to $3.86 \lesssim m_\pi L \lesssim 6.09$. Note that C005LV is simply a larger-volume version of C005, which provides a convenient test of volume dependence.

Label	$N_s^3 \times N_t$	a [fm]	DW Type	$am_{u,d}$	m_π [GeV]	$am_s^{\rm (sea)}$	$am_s^{\rm (val)}$	$N_{\rm ex}$	$N_{\rm sl}$
C00078	$48^3 \times 96$	0.114	Möbius	0.00078	0.13917(35)	0.0362	0.0362	158	5056
C005LV	$32^3 \times 64$	0.111	Shamir	0.005	0.3398(12)	0.04	0.0323	186	5022
C005	$24^3 \times 64$	0.111	Shamir	0.005	0.3398(12)	0.04	0.0323	311	9952
C01	$24^3 \times 64$	0.111	Shamir	0.01	0.4312(13)	0.04	0.0323	283	9056
F004	$32^3 \times 64$	0.083	Shamir	0.004	0.3036(14)	0.03	0.0248	251	8032
F006	$32^3 \times 64$	0.083	Shamir	0.006	0.3607(16)	0.03	0.0248	445	14240
F1M	$48^3 \times 96$	0.073	Möbius	0.002144	0.2320(10)	0.02144	0.02217	226	7232

Table 2: Parameters for the ensembles and domain-wall propagators used in this work.

The heavy quarks are handled with an anisotropic clover action tuned to remove discretization errors [28], which allow us to work directly at the physical charm and bottom masses for all lattice spacings. Our action is of the form

$$S_Q = a^4 \sum_x \bar{Q}\left[m_Q + \gamma_0\nabla_0 - \frac{a}{2}\nabla_0^{(2)} + \nu\sum_{i=1}^{3}\left(\gamma_i\nabla_i - \frac{a}{2}\nabla_i^{(2)}\right) - c_E\frac{a}{2}\sum_{i=1}^{3}\sigma_{0i}F_{0i} - c_B\frac{a}{4}\sum_{i,j=1}^{3}\sigma_{ij}F_{ij}\right]Q.$$

The bare mass am_Q, anisotropy coefficient ν, and clover coefficients $c_B = c_E$ are tuned by matching the $D_s^{(*)}$ and $B_s^{(*)}$ dispersion relations and hyperfine splittings [26, 29]. The values of these parameters are given in Ref. [26] (which labels the "C00078" ensemble "CP").

The currents used to calculate the decay constants are renormalized according to the mostly-nonperturbative method of Refs. [30, 31], and have the form

$$J_{V_0} = \sqrt{Z_V^{ss} Z_V^{QQ}}\rho_{V_0}\left[\bar{s}\gamma_0 Q + 2a\left(c^R_{V_0}\bar{s}\gamma_0\gamma_j\overrightarrow{\nabla}_j Q + c^L_{V_0}\bar{s}\overleftarrow{\nabla}_j\gamma_0\gamma_j Q\right)\right],$$
$$J_{A_i} = \sqrt{Z_V^{ss} Z_V^{QQ}}\rho_{A_i}\Big[\bar{s}\gamma_i\gamma_5 Q$$
$$+ 2a\left(c^R_{A_i}\bar{s}\gamma_i\gamma_5\gamma_j\overrightarrow{\nabla}_j Q + c^L_{A_i}\bar{s}\overleftarrow{\nabla}_j\gamma_i\gamma_5\gamma_j Q + d^R_{A_i}\bar{s}\gamma_5\overrightarrow{\nabla}_i Q + d^L_{A_i}\bar{s}\overleftarrow{\nabla}_i\gamma_5 Q\right)\Big].$$

Here, the factors Z^{qq} are computed nonperturbatively [21, 26, 32–34], while the residual matching factors ρ_J and $O(a)$-improvement terms are calculated to one loop in lattice perturbation theory [35, 36].

3. Operator Basis and Analysis

3.1 Operator Basis

To resolve the low-lying heavy-strange states of interest and compute the decay constants, we use the operator basis

$$\Phi^{(1)} = \bar{Q}s, \tag{1a}$$
$$\Phi^{(2)} = \bar{Q}\gamma^i\nabla_i s, \tag{1b}$$
$$J_{V_0} = \sqrt{Z_V^{ss} Z_V^{bb}}\rho_{V_0}\left[\bar{Q}\gamma_0 s + O(a)\text{-terms}\right], \tag{1c}$$
$$\Phi^{(4)}(\vec{x},t) = \sum_{\vec{y}}\Phi_K(\vec{x},t)\Phi_H(\vec{y},t) \ \text{ where } \Phi_K = \bar{u}\gamma_5 s,\ \Phi_H = \bar{Q}\gamma_5 u \tag{1d}$$

for $J^P = 0^+$, and

$$\Phi^{(1)i} = \bar{Q}\gamma^i\gamma_5 s, \tag{2a}$$
$$\Phi^{(2)i} = \bar{Q}\gamma_5\nabla^i s, \tag{2b}$$
$$J_{A_i} = \sqrt{Z_V^{ss} Z_V^{bb}}\rho_{A_i}\left[\bar{Q}\gamma_i\gamma_5 s + O(a)\text{-terms}\right], \tag{2c}$$
$$\Phi^{(4)i}(\vec{x},t) = \sum_{\vec{y}}\Phi_K(\vec{x},t)\Phi_{H^*}(\vec{y},t) \ \text{ with } \ \Phi_K = \bar{u}\gamma_5 s,\ \Phi_{H^*} = \bar{Q}\gamma^i u \tag{2d}$$

for $J^P = 1^+$. Inspecting Table 1 for the $J^P = 1^+$ charm case, we expect the quark-model spin triplet $D_{s1}(2460)$ to couple strongly to $\Phi^{(1)i}$, and the quark-model spin singlet $D_{s1}(2536)$ to couple strongly to $\Phi^{(2)i}$ — this will ultimately be what we find. For all systems, the two-meson operators $\Phi^{(4)(i)}$ are included to help resolve the $D^{(*)}K$ and $B^{(*)}K$ scattering states.

The light and strange quarks in all Φ fields are Gaussian-smeared using APE-smeared links, while the heavy quarks in the Φ fields are Gaussian-smeared using stout-smeared links.

Using the above operators, we compute zero-momentum-projected correlation matrices

$$C^{lm}(t) = \sum_{\vec{z}} \langle \Phi^{(l)}(\vec{z}, t + t_s) \Phi^{(m)\dagger}(\vec{x}_s, t_s) \rangle, \tag{3}$$

where $(\vec{x}_s, t_s)$ is the source position, and we use the convention that $\Phi^{(3)}$ corresponds to J_{V^0} or J_{A^i}.

From previous projects [26, 33, 34, 37] we have at our disposal precomputed light and strange quark propagators with Gaussian-smeared sources. To avoid having to compute new all-to-all light or strange propagators, we put the two-meson operators $\Phi^{(4)}$ only at the source. The elements $\sum_{\vec{z}} \langle \Phi^{(l)}(\vec{z}, t+t_s) \Phi^{(4)^\dagger}(\vec{x}_s, t) \rangle$ can then be computed using the light-quark propagator as a source for a sequential heavy-quark propagator, $T(z, x) \equiv \sum_{\vec{y}} G_Q(z; \vec{y}, t_s) \gamma_5 G_u(\vec{y}, t_s; \vec{x}_s, t_s)$. The correlation functions $\sum_{\vec{z}} \langle \Phi^{(l)}(\vec{z}, t + t_s) \Phi^{(2)^\dagger}(\vec{x}_s, t_s) \rangle$ with the derivative operators at the source are computed using heavy-quark propagators with derivative sources.

Where applicable, we average over Lorentz indices. We also average the off-diagonal C_{lm}'s with C_{ml}'s where both are available, as they have the same expectation values. Finally, we average over forward and backward propagation in time.

3.2 Data Analysis and Fitting

To determine the positive-parity spectra and decay constants, so far, we have focused on two different types of analyses. The first type combines a multi-exponential fit to the elements

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} \\ & C_{22} & C_{23} & C_{24} \\ & & C_{33} & C_{34} \end{pmatrix}, \tag{4}$$

without the $O(a)$ improvement terms in the currents, with another multi-exponential fit in which no currents are included at the source and instead the $O(a)$-improvement terms on their own are included at the sink. The reason for this approach is that the implementation of the $O(a)$-improvement terms in C_{l3} would require new strange-quark propagators with derivative sources.

The second type of analysis excludes the two-meson operators and uses single-exponential (for $J = 0$) or two-exponential (for $J = 1$) fits to the elements

$$\begin{pmatrix} C_{11} & \\ C_{21} & C_{22} \\ C_{31} & C_{32} \end{pmatrix}, \tag{5}$$

where the currents are included at the sink only and are fully $O(a)$-improved. The two-exponential fits are of the form $C_{ij} = A_i A_j \left(e^{-Et} + B_{1i} B_{1j} e^{-(E+\Delta E_1)t} \right)$ and are needed for $J = 1$ because of the additional low-lying spin-singlet energy level expected from the quark model. An example fit of C_{ij} and its associated effective-mass plot are exhibited below in Fig. 1. The decay constants of the ground states are obtained through $f = A_3 \sqrt{\frac{2}{E}}$.

In addition to the above analyses of the positive-parity heavy-strange systems, we extract the masses of the $H^{(*)} = D^{(*)}, B^{(*)}$ and K mesons that determine the strong-decay thresholds from single-exponential fits to simple two-point functions using quark-antiquark interpolating fields.

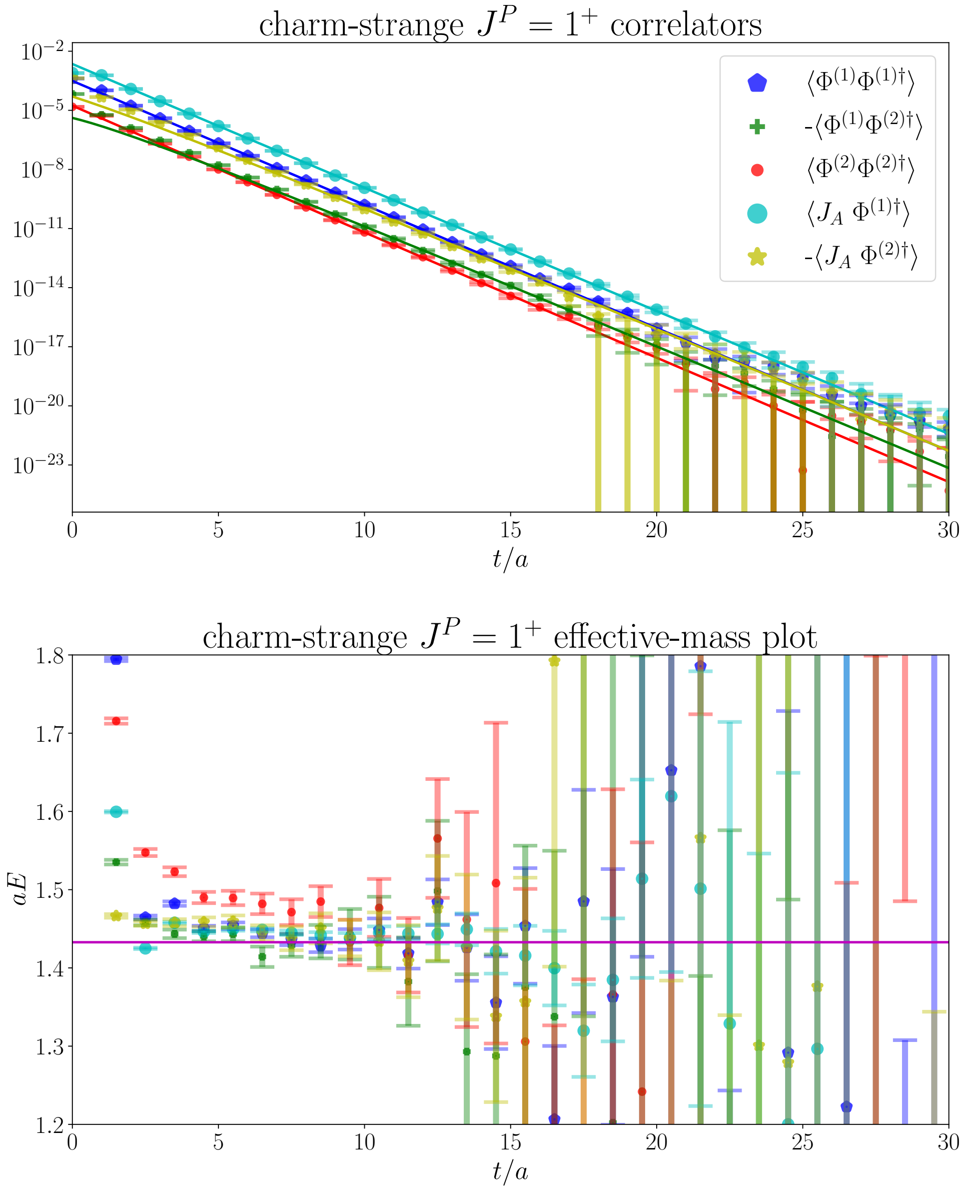

Figure 1: Correlation functions and corresponding effective-mass plot for the D_{s1}, fitted from $t_{\min}/a = 10$ to $t_{\max}/a = 16$ on the C00078 ensemble. The horizontal line shows the central value of fitted ground-state energy.

4. Results

The results presented at Lattice 2024 were obtained via the first type of analysis described in Sec. 3.2, with the two-meson operators included at the source. These fits were extremely unstable and led to unexpectedly low ground-state energies. It has been observed that correlation functions with two-hadron operators at one end only and local operators at the other end can lead to a negative bias in the fitted energy due to the emergence of false plateaus [38, 39]. We have since performed new fits using the second type of analysis without the two-meson operators and found these fits to be substantially more stable and have lower values of χ^2/d.o.f.. For this reason, we will only show the results from these new fits here. However, concerns remain that without the two-meson operators there may now be an overestimation of the ground-state energy levels.

Our results for the finite-volume "binding energies" $\Delta_H = E - E_{H^{(*)}} - E_K$ and decay constants extracted from the second type of analysis are plotted below in Figs. 2-3. The error bars are calculated by combining, in quadrature, the statistical uncertainties with an estimate of the systematic uncertainty due to the choice of $t_{\min}$, given by the shift in the central value when reducing $t_{\min}/a$ by 1.

The results for the B_{s0}^* and B_{s1} decay constants exhibit a surprisingly strong dependence on the lattice spacing, but we emphasize that the fit results may still be unreliable due to the exclusion of the two-meson operators.

We plan to revisit the fits with the two-meson operators included, and we are considering combining results from both fit types. We further intend to employ Lüscher's method [40] to extract infinite-volume bound state poles. Finally, we will perform chiral-continuum extrapolations of the results.

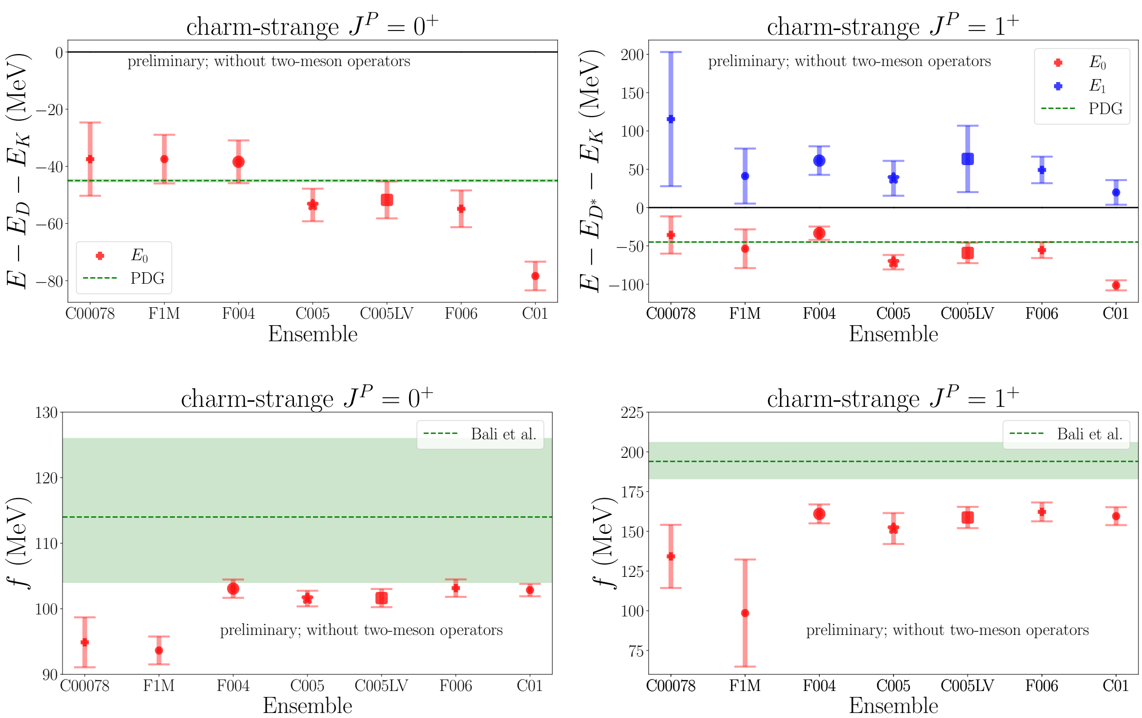

Figure 2: Finite-volume spectrum and decay constants of the D_{s0}^* and D_{s1}. For the spectrum, the bands show the experimental results for the ground state [20], and for the decay constants, the bands show the lattice results from Ref. [9].

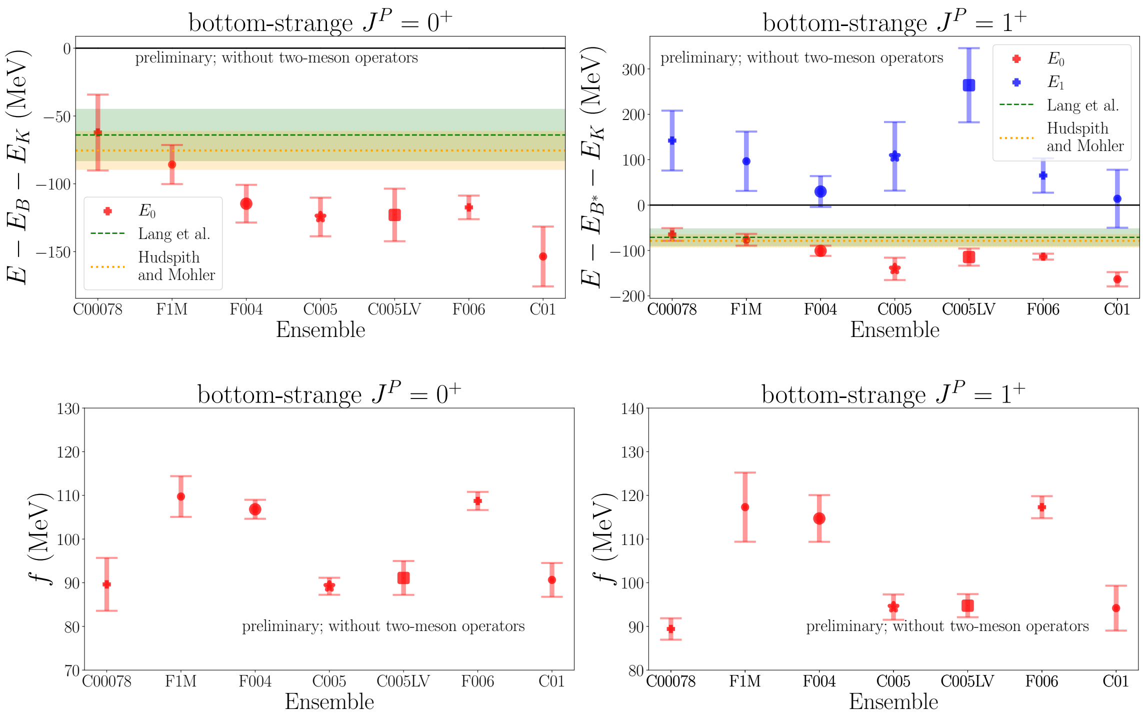

Figure 3: Finite-volume spectrum and decay constants of the B_{s0}^* and B_{s1}. Bands are infinite-volume estimates for the ground state from the lattice calculations of Refs. [13, 14].

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