Precise predictions of charmed-bottom hadrons from lattice QCD

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We report the ground state masses of hadrons containing at least one charm and one bottom quark using lattice quantum chromodynamics. These include mesons with spin (J)-parity (P) quantum numbers (JP): 0−, 1−, 1+ and 0+ and the spin-1/2 and 3/2 baryons. Among these hadrons only the ground state of 0− is known experimentally and therefore our predictions provide important information for the experimental discovery of all other hadrons with these quark contents.

PACS numbers: 12.38.Gc, 12.38.-t, 14.20.Lq

Recently heavy hadron physics has attracted huge scientific interests mainly due to the prospects of studying new physics beyond the Standard Model at the intensity frontier [1–5], and to study various newly discovered subatomic particles to better understand the confining nature of strong interactions [6–12]. From the perspective of newly found hadrons itself, a large number of discoveries over the past decade ranging from usual mesons [13–20], baryons [21] along with their excited states [22–25], to new exotic particles like tetraquarks [26–28] and pentaquarks [29], as well as hadrons whose structures are still elusive [30–33], have proliferated interests in the study of heavy hadrons. Furthermore, it is envisaged that the large data already collected or to be obtained at different laboratories, particularly at LHCb and Belle II, will further unravel many other hadrons. One variety of such theorized but as yet essentially unobserved (except one) subatomic particles are hadrons made of at least a charm and a bottom quarks, the charmed-bottom (bc) hadrons.

Investigations of such hadrons are highly appealing, as they provide a unique laboratory to explore the heavy quark dynamics at multiple scales: 1/mb, 1/me and 1/ΛQCD. Decay constants and form factors of bc mesons are still unknown but are quite important because of their relevance to investigate physics beyond the standard model, particularly in view of the recent measurement of R(J/ψ) [34]. The information on spin splittings and decay constants can shed light on their structures and help us to understand the nature of strong interactions at multiple scales. Moreover, bc baryon decays can aid in studying b → c transition and |Vcb| element of the CKM matrix.

However, to date the discovery of these hadrons is limited to only two observations: Bc(0−) with mass 6275(1) MeV [35] and Bc(2S)(0−) at 6842(6) MeV [36] while the latter has not yet been confirmed [37]. On the other hand, LHC being an efficient factory for producing bc hadrons [38–39], one would envisage for their discovery and study their decays in near future. Precise theoretical predictions related to the energy spectra and decay of these hadrons are thus utmost essential to guide their discovery.

In fact various model calculations exist in literatures on bc mesons [40–46] and baryons [47–53]. However, those predictions vary widely, e.g. 1S-hyperfine splitting in Bc(bc) mesons spread over a range of 40–90 MeV [40–46]. The predictions on bc baryons and excited states are even more scattered. Naturally first principle calculations using lattice QCD are quite essential to study these hadrons. However, unlike quarkonia, lattice study of bc hadrons are confined only to a few calculations [58–63]. In this work we carry out a detailed lattice calculation of the ground state energy spectra of all low lying bc hadrons (showed in Table 1) with very good control over systematics and predict their masses most precisely to this date.

| Mesons(q1q2) | Baryons ((q1q2q3)(JP)) |
|-------------|-------------------------|
| Bc(0−)     | Ξcb[cbu]                |
| Bc(1−)     | Ξcb[cbu]                |
| Bc(0+)     | Ωcb[cbu]                |
| Bc(1+)     | Ω∗cb[cbu]               |

TABLE I. List of bc hadrons that we study in this work. Quantum numbers (JP) along with the valence quark contents are also mentioned.

Lattice QCD studies are subject to various lattice artefacts. Of these the most relevant one in a study of heavy hadrons is the discretization error. It is thus essential to take a controlled continuum extrapolation of the results from finite lattice spacings. To that goal we obtain results at three lattice spacings: a = 0.12, 0.09 and 0.06 fm, and then are able to perform such extrapolations. Below we elaborate our numerical procedure.

Numerical details: A. Lattice ensembles: We use three dynamical 2+1+1 flavours (u/d, s, c) lattice ensembles generated by the MILC collaboration [67] with HISQ fermion action [68]. The lattices are with sizes 243 × 64, 323 × 96 and 483 × 96 at gauge couplings
10/g^2 = 6.00, 6.30 and 6.72, respectively [67]. The measured lattice spacings, obtained from \( r_f \) parameter, for the set of ensembles being used here are 0.1207(11) 0.08888(8) and 0.0582(5) fm, respectively [67].

**B. Quark actions:** For valence quark propagators, from light to charm quarks, we use the overlap action which has exact chiral symmetry at finite lattice spacings [69-71] and no \( O(\alpha_s) \) error. A wall source is utilized for calculating quark propagators.

For bottom quark we utilize a non-relativistic QCD (NRQCD) formulation [72] in which we incorporate all terms up to the leading term of the order of 1/\( M_0^3 \), where \( M_0 = a m_b \) is the bottom mass [73, 74]. This Hamiltonian is improved by including spin-independent terms through \( O(\alpha_s v^4) \) with non-perturbatively tuned improvement coefficients [77]. For the coarser two ensembles, we study the spectrum using "improved" coefficients as well as tree level coefficients ("unimproved").

**C. Quark mass tuning:** Following the Fermilab prescription for heavy quarks [80] we tune the heavy quark masses by equating the spin-averaged kinetic mass of the \( 1S \) quarkonia states (\( M_{\text{kin}}(1S) = \frac{3}{2} M_{\text{kin}}(1^-) + \frac{1}{2} M_{\text{kin}}(0^-) \)) to their physical values [76, 82]. A momentum induced wall-source, which is found to be very efficient compared to point or smeared sources [81], is utilized to obtain kinetic masses precisely. The tuned bare charm quark masses are found to be 0.528, 0.427 and 0.290 on coarse to fine lattices respectively, which also satisfy \( m_c a \ll 1 \), a necessary condition for reducing discretization effects. We tune strange quark mass, following Ref. [83].

**D. Hadron interpolators:** For mesons, we utilize the local meson interpolators (\( h \Gamma c \)), where \( \Gamma \), corresponding to different spin (J) and parity (P) quantum numbers, J^P, are: \( \gamma_5(0^-), \gamma_1(1^-), I(0^+) \) and \( \gamma_5 \gamma_1(1^+) \). We work with the assumption that the extracted ground state with \( \gamma_5 \gamma_1 \) is \( 1^+ \) and is unaffected by a possible nearby \( 2^+ \) level [58].

For baryons, we utilize the conventional interpolators given by \( P^*([\bar{c} q^T q]_3) \) as discussed in detail in Refs. [65, 66, 84]. For spin-1/2 \( \Xi_{cb} \) and \( \Omega_{cb} \), \( \Gamma = \gamma_5 \), whereas for spin-1/2 \( \Xi'_{cb} \), \( \Omega'_{cb} \) and spin-3/2 \( \Xi_{cb} \), \( \Omega_{cb} \) we use \( \Gamma = \gamma_i(i = 1, 2, 3) \) with appropriate spin projections.

A subtlety in the \( \Xi'_{cb} \) correlators is the possible admixture of \( \Xi_{cb} \) baryons. However, the use of wall source help us to clearly distinguish these two correlators which suggest that these two correlators coupled to two distinct states with no significant admixture. In the heavy quark limit, the total spin of the \( bc \) diquark becomes a good quantum number, and thus the mixing is heavily suppressed. An agreement between our results on these baryons with those obtained in Ref. [65] also justify this observation. Below we elaborate our results.

**Results:** To cancel out bare quark mass term which enters additively into the NRQCD Hamiltonian we calculate the mass differences between energy levels, rather than masses directly. To obtain the mass of a hadron (\( M_H \)) we first calculate subtracted masses on the lattice as

\[
\Delta M_H = |M_H^L - n_b \overline{\Delta S}_b/2 - n_c \overline{\Delta S}_c/2|a^{-1},
\]

where \( \overline{\Delta S}_b \) and \( \overline{\Delta S}_c \) are the lattice calculated spin average \( \overline{S} \) bottomonia and charmonia masses respectively, whereas \( n_b \) and \( n_c \) are the number of \( b \) and \( c \) valence quarks in the hadron. After calculating this subtracted mass we perform the continuum extrapolation to get its continuum value \( \Delta M_H^c \). Finally the physical result is obtained by adding the physical values of spin average masses to \( \Delta M_H^c \) as

\[
M_H = \Delta M_H^c + n_b (\overline{\Delta S}_b)_{\text{phys}} / 2 + n_c (\overline{\Delta S}_c)_{\text{phys}} / 2.
\]

Since the \( B_c(0^-) \) mass is known experimentally we also utilize a dimensionless ratio,

\[
R_H = \frac{M_H^c}{M_{B_c(0^-)}^c} - n_b \overline{\Delta S}_b / 2,
\]

which is then extrapolated to the continuum limit \( (R_H^c) \) and the final hadron mass is obtained from

\[
M_H^c = R_H^c \times (M_{B_c(0^-)} - n_b \overline{\Delta S}_b / 2)_{\text{phys}} + n_b (\overline{\Delta S}_b)_{\text{phys}} / 2.
\]

These procedures of utilizing dimensionless ratios as well as mass differences for the continuum extrapolations substantially reduce the systematic errors arising from mass tuning as well as for the terms which enter masses additively. We use both equations (2) and (4) and found consistent results and added the difference in systematics. Below we discuss results for \( bc \) mesons and baryons.

**Mesons:** In Figure 1 we plot the subtracted mass \( \Delta M_H \), as defined in Eq. (1), for \( B_c(0^-) \) as a function of lattice spacings \( (a) \). Blue circles represent unimproved and red squares represent improved results. We extrapolate unimproved results using fit forms \( Q^f = A + a^2 B \) as well as \( C^f = A + a^2 B \). Two bands corresponds to one

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**FIG. 1.** Ground state mass of the \( B_c(0^-) \) meson at three lattice spacings are plotted in terms of energy splittings from the spin-average mass (Eq(1)). Continuum extrapolated and experimental values are also shown.
sigma error for these fittings (purple: $Q^f$, green: $C^f$). The extrapolated result and the experimental value are shown by red and blue stars respectively. As expected the improved results are closer to the continuum limit (horizontal cyan bands show the proximity of the improved results from the continuum result). To see the consistency in fits we also use a constrained fit with both forms together by loosely constraining $A$ values from previous fits and difference in fitted parameters are included in discretization error. As in Figure 1 throughout we follow the same conventions for symbols and color coding. In Figure 2 (top), we plot the hyperfine splitting of $1S$ $B_c$ mesons. After the continuum extrapolation we obtain $B_c^+(1^−)−B_c^+(0^−)=55(3)$ MeV which is consistent with previous lattice calculations [58, 64] but more precise. In the bottom figure we show the subtracted ratios (Eq.(3)) and continuum extrapolations for the ground states of $1^−$, $1^+$ and $0^+$ $B_c$ mesons. Taking the experimental values for $B_c(0^−)$ and $1S$ quarkonia [55] masses, we obtain the ground state masses for these mesons and tabulate those in Table I.

**Baryons:** We first discuss the $\Xi_{cc}$ baryons. Presence of a valence light quark in $\Xi_{cc}$ demands a chiral extrapolation. Use of multimass algorithm allows to simulate a range of pion masses. In Figure 3 (top), we plot $\Xi_{cc}$ masses at various pion masses which clearly show a quadratic variation starting from the physical pion mass to ~ 600 MeV. We thus use a chiral extrapolation of the form $A + m^2 B$. Within the limit of acceptable $\chi^2$/dof, variations in chiral extrapolation forms, as in Ref. [65], do not change the final value. The same procedure is repeated for $\Xi_{cb}$ and $\Xi_{cb}^*$ at three lattices. These chiral extrapolated values are then used to calculate the subtracted masses and are plotted in the bottom part of Figure 3. These subtracted masses are then extrapolated to the continuum limit to get the ground state masses of these baryons and are tabulated in Table II. In Figs. 4 we show lattice extracted $\Delta M_H$ and the continuum extrapolations for different $\Omega$ baryons with flavor content $bcc$, $bqc$ and $bqc$, respectively. Continuum extrapolated results are shown by stars in each figure and are listed in Table III.

**Error estimation:** Below we address the estimation of various errors related to this work.

**Statistical:** The use of wall source reduces the statistical errors substantially and facilitates wide and stable fit ranges even for baryons. We find that the statistical error is always below percent level and is maximum for the $\Xi_{cc}$ baryons which is about 0.4%.

**Discretization:** Adaptation of overlap fermions ensures no $O(ma)$ error for light to charm quarks. The value of $ma$ for charm quarks (0.528, 0.427 and 0.290 on three lattices) are rather small compared to unity and hence implies smaller error from higher orders in $ma$. The utilization of energy splittings and ratios also ensure reduced systematics. This is clearly reflected in our estimates [76] for quarkonia hyperfine splittings ($\Delta E_{hfs}^{1S,cc} = 115(2)$)
TABLE II. Ground state masses of \( B_c \) mesons and baryons as predicted in this work. Statistical and systematic errors are shown inside two parentheses respectively.

| Hadrons       | Lattice  | Experiment |
|---------------|----------|------------|
| \( B_c(0^-) \) | 6276(3)  | 6274.9(8)  |
| \( B_c^*(1^-) \) | 6331(4)  | ?          |
| \( B_c(0^+) \) | 6712(18) | ?          |
| \( B_c(1^+) \) | 6736(17) | ?          |

\[ \Sigma_{a_b}(cbu)(1/2^+) = 6945(22)(14) \]
\[ \Sigma_{s_b}(cbu)(1/2^+) = 6966(23)(14) \]
\[ \Xi_{a_b}(cbu)(3/2^+) = 6089(24)(14) \]
\[ \Omega_{a_b}(cbu)(1/2^+) = 6994(15)(13) \]
\[ \Omega_{s_b}(cbu)(1/2^+) = 7045(16)(13) \]
\[ \Omega_{s_b}(cbu)(3/2^+) = 7056(17)(13) \]
\[ \Omega_{c_b}(1/2^+) = 8005(6)(11) \]
\[ \Omega_{c_b}(3/2^+) = 8026(7)(11) \]
\[ \Omega_{c_b}(1/2^+) = 11194(5)(12) \]
\[ \Omega_{c_b}(3/2^+) = 11211(6)(12) \]

FIG. 4. Subtracted masses, as defined in Eq. (1), of \( \Omega_{a_b}, \Omega_{s_b}^*, \Omega_a^* \) (top 3), \( \Omega_{c_b}, \Omega_{c_b}^* \) (middle 2), and \( \Omega_{c_b}, \Omega_{c_b}^* \) (bottom 2) baryons at three lattice spacings and at the continuum limit.

MeV and \( \Delta M_{b_c}^{1S,0S} = 63(3)(3) \) MeV). These splittings are known to be quite susceptible to this error and an excellent agreement between our and experimental values assures good control over discretization and hence a reliable estimation of masses of other heavy hadrons. Different fitting methods, quadratic, cubic in lattice spacing as well as both together in constrained fits, help to access possible discretization effects in continuum extrapolations. The largest discretization error is found to be for \( \Xi_{cb} \) baryons which is about 6-7 MeV.

Scale setting: We independently calculate lattice spacings from \( \Omega_{vass} \) baryon mass and found those to be consistent with the values measured by MILC collaboration [67]. The largest error in mass splittings due this scale uncertainty are within 6 MeV.

Finite size: The lattice volumes in this study is about 3 fm. Furthermore, the hadrons considered are quite heavy and are mostly stable to strong decays (there is no negative parity baryons). \( \Xi_{cb} \) baryons, only hadrons with valence light quark content, are found to have a perfect quadratic light quark mass dependence even towards the chiral limit indicating no observable finite size effects in them. Conservatively, we include a maximum uncertainty of a few MeV due to finite size effects, as estimated in Ref. [63] on similar lattice volume.

Chiral extrapolation: In this study only \( \Xi_{cb} \) baryons are subjected to this error. Due to the use of multmass algorithm we could calculate these baryons at a large number of pion masses, as shown in Figure 3 which help to perform extrapolations to the physical limit in a controlled and reliable way. Our results are found to be quite robust with respect to different chiral extrapolation forms.

NRQCD errors: Since we have included terms up to \( \alpha_s v^4 \), higher order terms, such as spin dependent as well as spin independent terms \( (\alpha_s^2 v^4 \) and \( \alpha_s v^6 \) will contribute to the systematics. For \( bc \) mesons, these errors are 4 MeV as estimated in Ref. [58] on similar lattices. As in Ref. [65], we also estimate these errors to be 5, 5 and 6 MeV for \( bcq, bbc \) and \( bbb \) baryons, respectively.

Other errors: Errors due to quark mass tuning are expected to be negligible in these results, considering the precision and rigor that enter into heavy quark mass tuning procedure. Use of wall source efficiently damps out excited state contamination providing long plateau in the effective mass at sufficiently large times indicating very good ground state saturation. Hence, any related uncertainties in our calculation are also negligible in comparison with any other errors. In a previous study we also found that the mixed action effects, which would vanish at the continuum limit, to be small [85] within this lattice set up. As discussed in Ref. [58], [83], [86] for similar lattices, the effect due to unphysical sea quark masses could be less than a percent level. Other errors due to electromagnetism, isospin breaking and the absence of dynamical bottom quarks are expected to be within 2-4 MeV [58].

As examples, following are the systematic error budget (in MeV) for \( B_c(0^-) \), \( \Omega_{c_b} \): discretization (3, 5), scale setting (2, 6), NRQCD errors (4, 7), finite volume (0, 2) and other sources (3, 5) which when are added in quadrature lead to systematic errors as \( \sim (6, 12) \) MeV.

Summary: In this Letter, we present precise predictions of the ground state masses of \( bc \) hadrons using lattice QCD simulations with very good control over sys-
ACKNOWLEDGEMENTS

We thank our colleagues within the ILGTI collaboration. We are thankful to the MILC collaboration and in particular to S. Gottlieb for providing us with the HISQ lattices. We would like to thank R. Lewis for helping with NRQCD code. We would also like to thank an unknown referee who has provided valuable comments on the mixing between $\Xi_{cb}$ and $\Xi'_{cb}$. Computations are carried out on the Cray-XC30 of ILGTI, TIFR, and on the Gaggle/Pride clusters of the Department of Theoretical Physics, TIFR. N. M. would like to thank Christine Davies for discussions and also to Ajay Salve and P. M. Kulkarni for computational supports. M. P. acknowledges support from EU under grant no. MSCA-IF-EF-ST-744659 (XQCDBaryons) and the Deutsche Forschungsgemeinschaft under Grant No.SFB/TRR 55.

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