Shallow Bound States and Hints for Broad Resonances with Quark Content $\bar{b}\bar{c}ud$ in $B-\bar{D}$ and $B^*-\bar{D}$ Scattering from Lattice QCD

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We present the first determination of the energy dependence of the $B-\bar{D}$ and $B^*-\bar{D}$ isospin-0, *S*-wave scattering amplitudes both below and above the thresholds using lattice QCD, which allows us to investigate rigorously whether mixed bottom-charm $\bar{b}\bar{c}ud$ tetraquarks exist as bound states or resonances. The scattering phase shifts are obtained using Lüscher's method from the energy spectra in two different volumes. To ensure that no relevant energy level is missed, we use large, symmetric 7×7 and 8×8 correlation matrices that include, at both source and sink, $B^{(*)}-\bar{D}$ scattering operators with the lowest three or four possible back-to-back momenta in addition to local $\bar{b}\bar{c}ud$ operators. We fit the energy dependence of the extracted scattering phase shifts using effective-range expansions. We observe sharp peaks in the $B^{(*)}-\bar{D}$ scattering rates close to the thresholds, which are associated with shallow bound states, either genuine or virtual, a few MeV or less below the $B^{(*)}-\bar{D}$ thresholds. In addition, we find hints for resonances with masses of order 100 MeV above the thresholds and decay widths of order 200 MeV.

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The majority of experimentally observed mesons can be understood in the quark model as quark-antiquark pairs. However, mesons, which are hadrons with integer spin, can in principle also be composed of two quarks and two antiquarks. The existence of these so-called tetraquarks had already been proposed in the early history of the quark model and QCD [1–3], but clear experimental confirmation was obtained only around a decade ago, for example in form of the observation of the charged Z_c and Z_b states as reviewed in Refs. [4,5]. While the masses and decays of the latter strongly indicate the presence of a $\bar{c}c$ pair or a $\bar{b}b$ pair, their nonvanishing electric charge implies additionally a light quark-antiquark pair. Recently, there was another experimental breakthrough in the field, namely the detection of the T_{cc} tetraquark with quark flavors $\bar{c}\bar{c}ud$ by LHCb [6,7]. In contrast to previously observed tetraquarks and tetraquark candidates, its mass is slightly below the lowest meson-meson threshold, making it by far the longest-lived experimentally confirmed tetraquark. Following the observation of this doubly charm tetraquark, possible next targets for experimental searches could be mixed bottom-charm tetraquarks with flavor content $\bar{b}\bar{c}ud$. Their production cross section at the LHC is estimated to be about 40 times larger compared to the doubly bottom $\bar{b}\bar{b}ud$ tetraquark [8]. The experimental signatures of a tetraquark are completely different depending on whether its mass is above or below the lowest strong-decay threshold. Thus, reliable theoretical predictions concerning $\bar{b}\bar{c}ud$ tetraquarks are very important and also urgent.

On the theoretical side, for the lightest $\bar{b}\bar{b}ud$ tetraquark with $I(J^P) = 0(1^+)$ (which is the bottom-quark partner of the previously mentioned T_{cc}), there is a consensus from recent lattice-QCD calculations that it is deeply bound [9–15] and will decay through the weak interaction only (see Refs. [8,16,17] for discussions of possible decay modes). For the case of $\bar{b}\bar{c}ud$, there is no such consensus.

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After finding initial hints for a possible QCD-stable $\bar{b}\bar{c}ud$ bound state with $I(J^P) = O(1^+)$ from lattice QCD [18], the same authors refined their calculation with larger lattice sizes and other improvements, and the hints disappeared [19]. In Ref. [13], some of us also performed lattice-QCD calculations of the $\bar{b}\bar{c}ud$ energy spectra for both $I(J^P) = O(1^+)$ and $I(J^P) = O(0^+)$, and we likewise did not find any evidence for OCD-stable bound states (although we could not *rule out* a shallow bound state). In contrast, another independent group very recently reported an $I(J^P) = O(1^+)$, $\bar{b}\bar{c}ud$ bound state $43\binom{+7}{-6}\binom{+24}{-14}$ MeV below the $B^* - \overline{D}$ threshold based on their lattice-QCD study [20], in which the $B^*-\bar{D}$ scattering length was determined using the Lüscher method [21–24] applied to the ground state. Nonlattice approaches also do not show a consistent picture. While Refs. [25–36] predict a QCD-stable $\bar{b}\bar{c}ud$ tetraquark, Refs. [37-42] reached the opposite conclusion.

In the following, we present a new lattice-QCD study of the $\bar{b}\bar{c}ud$ systems with both $I(J^P) = 0(1^+)$ and $I(J^P) = 0(0^+)$. This study uses a different lattice setup and substantially more advanced methods compared to previous work, allowing us to apply the Lüscher method to multiple excited states in addition to the ground state and hence to reliably determine the detailed energy dependence of the $B-\bar{D}$ and $B^*-\bar{D}$ isospin-0, *S*-wave scattering amplitudes.

In lattice QCD, the low-lying finite-volume energy levels with a given set of quantum numbers (the total spatial momentum, the quark flavor content, and the irreducible representation of the full octahedral group) are extracted from numerical results for imaginary-time two-point correlation functions $C_{ii}(t) = \langle \mathcal{O}_i(t) \mathcal{O}_i^{\dagger}(0) \rangle$. The operators \mathcal{O}_i are constructed out of quark and gluon fields such that they excite states with the desired quantum numbers, which resemble the low-lying energy eigenstates of interest. For an infinite (in practice, large) time extent of the lattice, the two-point function is equal to $C_{ij}(t) = \sum_{n} \langle \Omega | \mathcal{O}_i(0) | n \rangle \times$ $\langle n | {\cal O}_i^\dagger(0) | \Omega
angle \, e^{-E_n t}$, where $| \Omega
angle$ is the vacuum state and the sum is over all eigenstates $|n\rangle$ of the finite-volume OCD Hamiltonian for which the product of overlap matrix elements is nonzero. By analyzing the time dependence of the numerical results for $C_{ij}(t)$, the energies E_n can be extracted. Because lattice QCD uses a Monte-Carlo sampling of the Euclidean path integral, the numerical results have statistical uncertainties. Moreover, these uncertainties typically grow exponentially with t.

For multiquark systems, experience has shown that the simplest possible operator choices in which the quark fields are combined at the same spacetime point ("local" operators) are often insufficient to reliably extract even just the ground state [43]. The reason is that all or most of the energy levels resemble multihadron states with specific relative momenta, and the spectrum of such states in the case of heavy-quark systems is particularly dense. Among the previous lattice studies of $\bar{b}\bar{c}ud$ systems, Refs. [18–20] used only local four-quark operators with various types of smearing (local, wall, box) applied to each quark. Reference [13] improved upon this by including also two-meson ($B-\bar{D}$ and $B^*-\bar{D}$) "scattering" operators, that is, operators with each meson individually projected to a specific momentum (equal to zero only, in this case). These operators were included at the sink only, to avoid having to generate expensive all-to-all light-quark propagators. The work presented in the following no longer makes this restriction and is the first lattice-QCD calculation of $\bar{b}\bar{c}ud$ correlation matrices with $B^{(*)}-\bar{D}$ scattering operators at both source and sink, and also the first to include $B^{(*)}-\bar{D}$ scattering operators with nonzero back-to-back momenta.

Specifically, to study the $\bar{b}\bar{c}ud$ system with $I(J^P) =$ $0(0^+)$, we use seven operators $\mathcal{O}_{1...7}^{A_1^+}$, of which $\mathcal{O}_1^{A_1^+}$ through $\mathcal{O}_3^{A_1^+}$ are operators with all four quarks at the same spacetime point (but with Gaussian smearing of the quark fields) and jointly projected to zero total spatial momentum, and $\mathcal{O}_4^{A_1^+}$ through $\mathcal{O}_7^{A_1^+}$ are $B \text{-} \bar{D}$ scattering operators with zero total spatial momentum in which the B and \overline{D} operators have back-to-back momenta of magnitudes 0, $2\pi/L$, $\sqrt{2} 2\pi/L$, and $\sqrt{3} 2\pi/L$ (*L* is the spatial lattice size). Similarly, for the $\bar{b}\bar{c}ud$ system with $I(J^P) = O(1^+)$, we use eight operators $\mathcal{O}_{1...8}^{T_1^+}$, of which $\mathcal{O}_1^{T_1^+}$ through $\mathcal{O}_4^{T_1^+}$ are local four-quark operators and $\mathcal{O}_5^{T_1^+}$ through $\mathcal{O}_8^{T_1^+}$ are $B^* \cdot \bar{D}$ scattering operators in which the B^* and \bar{D} have backto-back momenta of magnitudes 0, $2\pi/L$ (for both $\mathcal{O}_6^{T_1^+}$ and $\mathcal{O}_7^{T_1^+}$), and $\sqrt{2} 2\pi/L$. Two different operators are used for the case with one unit of back-to-back momentum to account for the mixing of S and D partial waves [44]. The labels A_1^+ and T_1^+ refer to the octahedral-group irreps of positive parity that contain the angular momenta $J = 0, 4, \dots$ and $J = 1, 3, \dots$, respectively. The explicit definitions of all operators are given in the Supplemental Material [45]. We compute the symmetric 7×7 and 8×8 correlation matrices of these operators, using combinations of (Gaussian smeared) point-to-all and stochastic time slice-to-all propagators [53].

Our calculations were performed for two different lattice sizes, $24^3 \times 64$ and $32^3 \times 64$, with a lattice spacing of approximately 0.12 fm and pion mass of approximately 220 MeV in both cases. The charm and bottom valence quarks were implemented using the Fermilab method [54] and lattice NRQCD [55], respectively, with approximately physical kinetic masses. Further details are provided in the Supplemental Material.

We computed the $\bar{b}\bar{c}ud$ correlation matrices for approximately 1000 gauge configurations on each lattice, with 30 source locations per configuration for the elements computed using (Gaussian smeared) point-source propagators, and three random $\mathbb{Z}_2 \times \mathbb{Z}_2$ sources on four time slices per



FIG. 1. Left: the finite-volume energies of the $\bar{b}\bar{c}ud$ system with $I(J^P) = 0(0^+)$ as a function of the spatial lattice size. The data points with error bars show the actual finite-volume energy levels; points plotted with a lighter shade of gray are excluded from the Lüscher analysis. The solid blue curves correspond to what would be the noninteracting $B-\bar{D}$ energy levels, the lowest of which coincides with the strong-decay threshold. The dashed green line shows the $B^*-\bar{D}^*$ threshold. Right: the correspond to what would be the noninteracting $B^*-\bar{D}$ energy levels, and the dashed green line corresponds to the $B^*-\bar{D}^*$ threshold. Right: the correspond to what would be the noninteracting $B^*-\bar{D}$ energy levels, and the dashed green line corresponds to the $B-\bar{D}^*$ threshold.

configuration for the elements computed with (Gaussian smeared) stochastic propagators; we also use color and spin dilution and the one-end trick [53]. To extract the $\bar{b}\bar{c}ud$ finite-volume energy levels from these correlation matrices, we follow the well-established approach of solving the generalized eigenvalue problem (GEVP) [22,56]

$$\sum_{j} C_{ij}(t) v_{j,n}(t,t_0) = \lambda_n(t,t_0) \sum_{j} C_{ij}(t_0) v_{j,n}(t,t_0), \quad (1)$$

where we set $t_0/a = 3$ and verified that the results do not significantly depend on this choice. We then perform single-exponential fits of the form $\lambda_n(t, t_0) = A_n e^{-E_n t}$ to obtain the energy levels E_n ; see the Supplemental Material [45] for further details.

Our results for the lowest five energy levels of each $\bar{bc}ud$ system are shown as a function of the spatial lattice size $N_s = L/a$ in Fig. 1. Also shown are the lowest four noninteracting $B^{(*)}-\bar{D}$ energy levels, calculated as $E = E_{B^{(*)}}(\mathbf{p}^2) + E_{\bar{D}}(\mathbf{p}^2)$ with momenta \mathbf{p} satisfying the periodic boundary conditions [each component an integer multiple of $2\pi/L$], and with the single-meson energies calculated on the lattice and described by the dispersion relations

$$E_{B^{(*)}}(\mathbf{p}^2) = E_{B^{(*)}}(0) + \sqrt{m_{B^{(*)},\rm kin}^2 + \mathbf{p}^2} - m_{B^{(*)},\rm kin},$$

$$E_D(\mathbf{p}^2) = E_{\bar{D}}(0) + \mathbf{p}^2 / (2m_{\bar{D},\rm kin}) - \mathbf{p}^4 / (8m_{\bar{D},4}^3).$$
(2)

The values of $E_{B^{(*)}}(0)$, $m_{B^{(*)},kin}$, $E_{\bar{D}}(0)$, $m_{\bar{D},kin}$, and $m_{\bar{D},4}$ are provided in the Supplemental Material [45]. In Fig. 1 we see that the actual $\bar{b}\bar{c}ud$ energy levels are shifted significantly relative to the noninteracting levels due to the meson-meson interactions in the finite volume, except for the third level in the case of J = 1 (we discuss the reason for this behavior farther below).

To rigorously investigate whether bound states or resonances exist, we map the observed finite-volume energy levels E_n to infinite-volume *S*-wave $B^{(*)}$ - \overline{D} scattering phase shifts $\delta_0(k_n)$ using the Lüscher quantization condition

$$\cot \delta_0(k_n) = \frac{2Z_{00}[1; (k_n L/2\pi)^2]}{\pi^{1/2} k_n L},$$
(3)

where Z_{00} is the generalized zeta function [23] and k_n is the scattering momentum associated with energy level E_n , calculated from $E_n = E_{B^{(*)}}(k_n^2) + E_{\bar{D}}(k_n^2)$ with the dispersion relations (2). To ensure that the single-channel, single-partial-wave approximation is applicable, we only extract the phase shifts for the energy levels below the $B^* - \bar{D}^*$ (J = 0) and $B - \bar{D}^*$ (J = 1) thresholds. Furthermore, for J = 1, we observe that the third finite-volume energy level is consistent with the noninteracting $|\mathbf{p}| = 2\pi/L$ energy level that has multiplicity 2 once we include both S-wave and D-wave structures, as we did in our operator basis. Because finite-volume interactions for higher partial waves are suppressed, we conclude that this energy level is dominantly D wave, and we therefore exclude it from the Lüscher analysis. This is further corroborated by the eigenvectors from the GEVP, which show that this state has a non-negligible overlap only with the operator $\mathcal{O}_{7}^{T_{1}}$ that was subduced from a D-wave structure. Note that there are similar degeneracies for higher noninteracting levels above the energy region used in our analysis [44].

Our results for the scattering phase shifts, along with effective-range expansion (ERE) fits of the form

$$k\cot\delta_0(k) = \frac{1}{a_0} + \frac{1}{2}r_0k^2 + b_0k^4,$$
(4)

are shown in Fig. 2 (left). The numerical values of the fitted ERE parameters are given in the Supplemental Material [45]. The scattering phase shift is related to the *S*-wave scattering amplitude and cross section by

$$T_0(k) = \frac{1}{\cot \delta_0(k) - i}, \qquad \sigma(k) = \frac{4\pi}{k^2} |T_0(k)|^2.$$
(5)

Poles of $T_0(k)$ at purely imaginary k correspond to genuine or virtual bound states for Im(k) > 0 or Im(k) < 0, respectively, while poles with $\text{Re}(k) \neq 0$ and Im(k) < 0correspond to resonances. Using our ERE fits, we find genuine bound-state poles as well as resonance poles for



FIG. 2. Left: our results for the functions $ak \cot \delta_0(k)$ for *S*-wave $B \cdot \bar{D}$ scattering (top) and *S*-wave $B^* \cdot \bar{D}$ scattering (bottom), where *k* is the scattering momentum, $\delta_0(k)$ is the scattering phase shift, and a = 0.11887(80) fm is the lattice spacing. The data points were obtained directly from the lattice energy levels, and the curves correspond to ERE fits through order k^4 . Also shown are the functions $-\sqrt{-(ak)^2}$ (solid red parabolas) whose intersections with $ak \cot \delta_0(k)$ just below threshold correspond to the shallow $\bar{b}\bar{c}ud$ bound states we predict, and $+\sqrt{-(ak)^2}$ (dashed red parabolas) whose intersections with $ak \cot \delta_0(k)$ would correspond to virtual $\bar{b}\bar{c}ud$ bound states. The vertical magenta lines show the positions of two-pion-exchange left-hand branch points. Right: our results for the product of scattering momentum and $B^{(*)} \cdot \bar{D}$ scattering cross section, which is proportional to the scattering rate, as a function of center-of-momentum energy.

both J = 0 and J = 1 at the values of $\sqrt{s} - \sqrt{s_{\text{th}}} = \sqrt{m_{B^{(*)}}^2 + k^2} + \sqrt{m_{\bar{D}}^2 + k^2} - m_{B^{(*)}} - m_{\bar{D}}$ given in Table I (*s* denotes the Mandelstam variable equal to the square of the center-of-momentum energy). We used our lattice results for the kinetic $B^{(*)}$ and \bar{D} masses to evaluate this expression; to obtain predictions for absolute tetraquark bound state or resonance masses, one simply needs to add the experimental value of the threshold energy, $m_{B^{(*)}}^{\exp} + m_{\bar{D}}^{\exp}$.

The resonances have masses of order 100 MeV above the $B^{(*)}-\bar{D}$ thresholds and decay widths of order 200 MeV. We caution that the resonance poles lie outside the radius of convergence of the ERE, which is limited by the presence of a left-hand cut associated with a two-pion *t*-channel exchange in the scattering process (a single-pion exchange would require a D^* in the initial or final state, and is therefore not relevant here). The center-of-momentum energy at which the left-hand cut starts is obtained from the kinematic relations for the Mandelstam variables by expressing *s* in terms of *t* and the scattering angle θ^* , and

then setting $t = (2m_{\pi})^2$ and $\theta^* = \pi$ [57]; this gives $\sqrt{s_{\text{cut}}}$ – $\sqrt{s_{\text{th}}} \approx -18$ MeV for both J = 0 and J = 1, corresponding to $(ak)_{cut}^2 \approx -0.019$, as indicated with the magenta lines in Fig. 2. While our ERE fit is seen to describe the data very well for real $(ak)^2$ in the full momentum range, the prediction of resonance poles away from the real axis may be less reliable. We note, however, that instead of expanding $k \cot \delta_0(k)$ around $k^2 = 0$ one could as well expand around the midpoint of the left-hand cut and the second threshold. The convergence radius in the complex energy plane would then be significantly larger, while the resulting parametrizations of the lattice data points for $k \cot \delta_0(k)$ would be identical to those obtained from the ERE. The reason is that in both cases second-order polynomials in k^2 are fitted to the same data points. This suggests that our results can be trusted in a significantly larger region of the complex energy plane, namely disks of radius 94 MeV around E = 76 MeV for J = 0 and of radius 52 MeV around E = 34 MeV for J = 1. The predicted resonances are still located outside, but quite close to the boundaries of these convergence regions. To further test their stability, we also performed ERE fits

TABLE I. Our results for the $\bar{b}\bar{c}ud$ genuine-bound-state (GBS) and resonance (*R*) pole locations, where $\Delta m_{\text{GBS}} = m_{\text{GBS}} - m_{\bar{b}}, \Delta m_R = \text{Re}(\sqrt{s_R}) - m_{\bar{b}}, \text{and } \Gamma_R = -2\text{Im}(\sqrt{s_R}).$ Only the statistical uncertainties are given.

	$\Delta m_{\rm GBS}$ [MeV]	$\Delta m_{\rm R}$ [MeV]	$\Gamma_{\rm R}$ [MeV]
J = 0	$-0.5^{+0.4}_{-1.5}$	138(13)	229(35)
J = 1	$-2.4^{+2.0}_{-0.7}$	67(24)	132(32)

through order k^6 . The coefficients of k^6 are found to be consistent with zero within the statistical uncertainties, and the other parameters remain consistent with those from the order- k^4 fit. For J = 0, the resonance pole obtained from the order- k^6 fit is at a similar location. For J = 1, where we have fewer data points, the uncertainties from the k^6 fit are too large to determine the pole locations.

The bound-state poles are extremely close to threshold and therefore well within the region of validity of the ERE. However, as can be seen from the $\pm \sqrt{-(ak)^2}$ parabolas in Fig. 2, statistical fluctuations could turn the genuine bound states into virtual bound states, which are not asymptotic states in QCD but would still strongly affect the $B^{(*)}-\bar{D}$ scattering rates near threshold [58], or could, at first glance, lead to the complete disappearance of the poles. To quantify this uncertainty, we generated 10 000 multivariate Gaussian random samples for the ERE fit parameters a_0 , r_0 , and b_0 according to their mean values and covariance matrix. For each sample, we first checked whether it is still consistent with our finite-volume energy spectra. To this end, we calculate the two finite-volume energy spectra predicted by the sample using the Lüscher quantization condition. For some of the samples, the intersection of $k \cot \delta_0(k)$ and $2Z_{00}[1; (k_n L/2\pi)^2]/(\pi^{1/2}L)$ below threshold disappears for at least one of the volumes, leaving only the intersections that match the first and higher excited-state energy levels calculated on the lattice. These samples are therefore inconsistent with the observed spectra, and we removed them. For each of the remaining samples, we then checked whether there is a genuine bound state (GBS), a virtual bound state (VBS), or no bound state (NBS), with the following outcome: J = 0: 88.5% GBS, 11.5% VBS, 0.0% NBS; and *J* = 1: 97.7% GBS, 2.3% VBS, 0.0% NBS.

The lower and upper limits for Δm_{GBS} given in Table I correspond to the 16th and 84th percentiles of those random samples for which genuine bound states exist, while the central values correspond to the best-fit points. To further test our prediction of shallow bound states, we performed additional ERE fits of order k^0 and order k^2 using only the three data points closest to threshold, which are within the strict radius of convergence of the ERE. These fits, which are shown in the Supplemental Material [45], give consistent results.

Returning to the discussion of our main fits as shown in Fig. 2, we note that, in addition to the shallow-bound-state

and the broad-resonance poles, there are poles with purely imaginary k below the left-hand branch point. These poles must be discarded because the direction of the crossing corresponds to a pole residue with an unphysical sign [59], and our parametrization of $k \cot \delta_0(k)$ is invalid in that region (bound states this far below threshold are also ruled out by the absence of corresponding finite-volume energy levels).

The scattering rate (probability per time) is equal to the product of flux and cross section, and hence proportional to $k\sigma(k)$ for nonrelativistic k. These products are shown in Fig. 2 (right) as a function of the center-of-momentum energy. We emphasize that the scattering rates only depend on our fit functions for real-valued k^2 that interpolate our data very well, so these predictions are also expected to be very reliable. We observe sharp enhancements in the scattering rates close to the thresholds, related to the shallow bound states or virtual bound states. At higher energies, the scattering rates continue to be enhanced, likely by the broad resonances. The scattering rates are very close to the largest possible value allowed by unitarity, given by $|T_0|^2 = 1$, up to several tens of MeV above threshold.

In summary, the substantial improvements made here in determining the $\bar{b}\bar{c}ud$ finite-volume energy levels allowed us to determine the detailed energy dependence of the $B-\bar{D}$ and $B^* - \overline{D}$ S-wave scattering amplitudes for the first time using lattice QCD, revealing very interesting stronginteraction phenomena. We found poles for both J = 0and J = 1 corresponding to shallow bound states, as well as hints for poles corresponding to broad resonances. While further lattice-QCD computations at additional lattice spacings and pion masses will be needed to pin down the exact location and nature of each pole at the physical point, we expect our prediction of shallow bound states, either genuine or virtual, to be quite robust. The possible resonances above threshold are very broad and are therefore presumably difficult to observe at the LHC and future experiments. On the other hand, if the J = 0 pole just below the $B-\bar{D}$ threshold is confirmed as a genuine bound state, this isoscalar, scalar $\bar{b}\bar{c}ud$ tetraquark will decay through the weak interaction only and could become the first tetraquark to be observed at the LHC with this feature. If the J = 1 pole just below the $B^*-\bar{D}$ threshold is confirmed as a genuine bound state, it will decay electromagnetically into $B\bar{D}\gamma$ (and also into the J = 0 tetraquark plus a photon, if that tetraquark is confirmed as a genuine bound state).

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