Zb tetraquark channel from lattice QCD and Born-Oppenheimer approximation

S. Prelovsek,1,2,3 H. Bahtiyar,2,4 and J. Petkovic1,2

1Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia
2Jožef Stefan Institute, Ljubljana, Slovenia
3Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany
4Department of Physics, Mimar Sinan Fine Arts University, Bomonti 34380, Istanbul, Turkey

Two Zb hadrons with exotic quark structure bbdu were discovered by Belle experiment. We present a lattice QCD study of the bbdu system in the approximation of static b quarks, where the total spin of heavy quarks is fixed to one. The energies of eigenstates are determined as a function of separation r between b and b. The lower eigenstates are related to a bottomonium and a pion. The eigenstate dominated by BB* has energy significantly below mb + mb*, which points to sizable attraction for small r. The attractive potential V(r) between b and b* is extracted assuming that this eigenstate is related exclusively to BB*. The Schrödinger equation for BB* within the extracted potential leads to a virtual bound state, whose mass depends on the parametrization of the lattice potential. For certain parametrizations, we find a virtual bound state slightly below BB* threshold and a narrow peak in the BB* rate above threshold - these features could be related to Zb(10610) in experiment. We surprisingly find also a deep bound state within undertaken approximations.

The Belle experiment discovered two Zb+ states with exotic quark content bbdu, JP = 1+ and I = 1 in 2011 [11, 12] and is reviewed below. No other lattice results are available since this channel presents a severe challenge. Scattering matrix would have to be determined using the Lüscher method for at least 7 coupled channels listed in the previous paragraph. Poles of scattering matrix would render possible Zb states. Following this path seems too challenging at present.

In the present study we consider the Born-Oppenheimer approximation [20], inspired by the study of this system in [18, 19]. It is applied in molecular physics since ions are much heavier than other degrees of freedom. It is valuable also for the Zb system bbdu, where b and b represent heavy degrees of freedom (h), while light quarks and gluons are light degrees of freedom (l), see for example [21, 22]. The simplification comes from the fact that heavy degrees of freedom have large mass and therefore small velocity and kinetic energy.

In the first step we treat b and b as static at fixed distance r (Figure 1a) and the main purpose is to determine eigen-energies En(r) of this system. This energy represents the total energy without the kinetic and rest energies of the b and b, so En(r) is related to the potential V(r) felt by the heavy degrees of freedom. In the second step, we study the motion of the heavy degrees of freedom (with physical masses) under the influence of the extracted potential V(r). Solutions of the Schrödinger equation render information on possible (virtual) bound states Zb, resonances and cross-sections.

The low-lying eigenstates of the system in Fig. 1a and quantum numbers (2) are related to two-hadron states in Figs. 1(b-d)

\[ B(0)B^*(r), \, \Upsilon(r)\pi(\bar{p} = 0), \, \Upsilon(r)\pi(\bar{p} \neq 0), \, \Upsilon(r)b_1(\bar{0}). \] (1)

The eigen-energy En(r) related to BB* in Fig. 1 is of most interest since Zb lie near BB* threshold. Bottomonium-pion states Υ(r)π(\bar{p}) represent ground state at small r. Here Υ(r) denotes spin-one bottomonium where b and b are separated by r. Pion can have zero or non-zero momentum \(\bar{p} = \vec{n} \frac{2\pi}{r}\) since total momenta of light degrees of freedom is not conserved in the presence of static quarks, i.e. pion momentum can change when it scatters on infinitely heavy Υ. Our task is to extract energies of all these eigenstates E_n(r) as a function of separation r. The only previous lattice study of this system [18] presents preliminary results based on Fock components BB* and Υπ(0); the presence Υπ(\bar{p} \neq 0) was mentioned in [19], but not included in the simulation.

Quantum numbers and operators: We consider Zb that has quantum numbers I = 1, I_3 = 0, J_{PC} = 1^{-+} and J_z = 0 in experiment. The list of conserved quantum numbers is slightly different in the systems with two static particles. We study the system in Fig. 1a with quantum numbers

\[ I = 1, \, I_3 = 0, \, \epsilon = -1, \, C \cdot P = -1 \] (2)

\[ S^h = 1, \, S_z^h = 0, \, J_z = 0, \, (h = heavy, \, l = light) \]

where the neutral system is considered so that C-conjugation can be applied (Fig. 1d shows the charged partner). Only the z-component of angular momenta for
light degrees of freedom ($J_{z}^{light}$) is conserved. The quantum number $\epsilon$ corresponds to the reflection over the yz plane. $P$ refers to inversion with respect to mid-point between $b$ and $\bar{b}$ and $C$ is charge conjugation, where only their product is conserved.

The spin of the infinitely heavy quark can not flip via interaction with gluons, so spin $S^h$ of $b\bar{b}$ is conserved. We choose to study the system with $S^h = 1$, which can decay to $\Upsilon$, while it can not decay to $\eta_b$ and $b_b$ since these carry $S^h = 0$. Note that the physical $Z_b$ and $B^*B^*$ with finite $m_b$ can be a linear combination of $S^h = 1$ as well as $S^h = 0$, and we study only $S^h = 1$ component here. We have in mind this component, which includes $BB^*$, $\bar{B}B^*$, $B^*B^*$ ($O_1$ in Eq. 3), when we refer to "BB$^*$" throughout this paper.

The eigen-energies $E_n$ of the system in Fig. 1a are determined from the correlation functions ($O_i(t)O_i^\dagger(0)$). We employ 6 operators $O_i$ that create/annihilate the system with quantum numbers $|2\rangle$ and resemble Fock components $|1\rangle$ in Figs. 1(b-d)

$$O_1 = O^{BB^*} \propto \sum_{a,b} \sum_{A,B,C,D} \Gamma_{BA} \bar{b}^b_A(0) q^A_0 \langle 0 | \bar{b}^b(r) b^b(r)$$

$$\propto (\bar{b}(0) P_\gamma q(0)) |q(r) \gamma_+ P_\gamma b(r) + \{ \gamma_+ \leftrightarrow \gamma_2 \}$$

$$+ (\bar{b}(0) P_\gamma q(0)) |q(r) \gamma_+ P_\gamma b(r) - \{ \gamma_9 \leftrightarrow \gamma_2 \})$$

$$O_2 = O^{B^*}\bar{B}$$

$$O_3 = O^{T\pi(0)} \propto \bar{b}(0) U \gamma_+ P_\gamma b(r) |q(\gamma_5)\gamma_5 \rangle_{\vec{p}=0}$$

$$O_4 = O^{T\pi(1)} \propto \bar{b}(0) U \gamma_+ P_\gamma b(r) (|q(\gamma_5)\gamma_5 \rangle_{\vec{p}=\vec{e}} + |q(\gamma_5)\gamma_5 \rangle_{\vec{p}=-\vec{e}})$$

$$O_5 = O^{T\pi(2)} \propto \bar{b}(0) U \gamma_+ P_\gamma b(r) (|q(\gamma_5)\gamma_5 \rangle_{\vec{p}=2\vec{e}} + |q(\gamma_5)\gamma_5 \rangle_{\vec{p}=-2\vec{e}})$$

$$O_6 = O^{Tb_1(0)} \propto \bar{b}(0) U \gamma_+ P_\gamma b(r)|q(\gamma_5)\gamma_5 \rangle_{\vec{p}=0}.$$

Here $\Gamma=P_\gamma \gamma_5$, $\bar{\Gamma}=\gamma_5 P_\gamma$, $[\Gamma' q(\vec{x})]_{\vec{p}} = \frac{1}{r} \sum_{n} \bar{q}(\vec{x}) \Gamma' q(\vec{x}) e^{i \vec{p} \cdot \vec{x}}$, momenta is given in units of $2\pi/L$, capital (small) letters represent Dirac (color) indices, color singlets are denoted by $[…]$, and $U$ is a product of gauge links between 0 and $r$. First line in $O_1$ decouples spin indices of light and heavy quarks, so that $J_z^L$ and $S_{z}^{(c)}$ are more transparent, while the second line is obtained via Fierz transformation. $O_2$ is obtained from $O_1$ by replacing all $q(x)$ with $\nabla q(x)$. $O_{4,5}$ have pion momenta in $z$ direction due to $J_z^L = 0$ and have two terms to ensure $C \cdot P = -1$. The $Tb_1$ is not a decay mode for finite $m_b$ where $C$ and $P$ are separately conserved, but it is has quantum numbers $|2\rangle$ for $m_b \to \infty$. The pair $\bar{q}q$ indicates combination $uu-\bar{u}d$ with $I = 1$ and $I_3 = 0$. All light quarks $q(x)$ are smeared around position $x$ using full distillation with radius about 0.3 fm, while heavy quarks are point-like.

We verified there are no other two-hadron states in addition to $|1\rangle$ with quantum numbers $|2\rangle$ and with non-interacting energies $|1\rangle$ below $m_B + m_{B^*} + 0.2$ GeV.

**Lattice details:** Simulation is performed on an ensemble with dynamical Wilson-clover $u/d$ quarks, $m_\pi \approx 266(5)$ MeV, $a \approx 0.1239(13)$ fm and 280 configurations $|24\rangle$ $|25\rangle$. We choose an ensemble with small $N_L = 16$ and $L \approx 2$ fm so that $\Upsilon(\vec{p})$ with $p_c > 2\pi$ appear as $E > m_B + m_{B^*} + 0.2$ GeV above our interest; larger $L$ would require further operators like $O_{4,5}$ with higher $\vec{p}$.

**Calculation of eigen-energies and overlaps:** Correlation matrices $C_{ij}(t) = \langle O_i(t)O_i^\dagger(0) \rangle$ are evaluated using the full distillation method $|24\rangle$ and $bb$ annihilation Wick contraction is omitted as in practically all quarkonium lattice studies. $C_{ij}$ are averaged over $8^3$ or $16^3$ space positions of $b$, while sub-matrix for $O_{3-6}$ is averaged over all source time slices to increase accuracy. Eigen-energies $E_n$ and overlaps $\langle O_i | n \rangle$ are extracted from 6 $\times$ 6 matrices $C_{ij}(t) = \sum_n \langle O_i | n \rangle e^{-E_n t}(O_j | n \rangle)$ using the widely used GEVP variational approach $|26\rangle$ $|28\rangle$.

**Eigen-energies of $bb\bar{d}u$ system as a function of $r$:** The main result of our study are the eigen-energies of the $bb\bar{d}u$ system (Fig. 1a) with static $b$ and $\bar{b}$ separated by $r$. They are shown by points in Figure 2. The colors of points indicate which Fock-component ($|1\rangle$) dominates an eigenstate, as determined from normalized overlaps of an eigenstate $|n \rangle$ to operators $O_i$. Normalized overlap $\bar{Z}_n = |\langle O_i | n \rangle | / \max_m |\langle O_i | m \rangle |$ is normalized so that its maximal value for given $O_i$ across all eigenstates is equal to one.

The dashed lines in Fig. 2 provide related non-interacting (n.i.) energies $E_n$ of two-hadron states $|1\rangle$

$$E_{B^*B}^{n.i.} = 2m_B, \ E_{\pi(\vec{p})}^{n.i.} = \frac{V_{bb}(r) + E_{\pi(\vec{p})}}{V_{bb}(r) + m_{b}}, \ E_{Tb_1(0)}^{n.i.} = V_{bb}(r) + m_b,$$

where $bb$ static potential $V_{bb}(r)$, $E_{\pi(\vec{p})} \approx \sqrt{m_b^2 + \vec{p}^2}$, $m_b$, and $m_{b} = m_{B^*}$ (mass of $B^*(c)$ for $m_b \to \infty$ without $b$ rest mass) are determined on the same ensemble.

The eigenstate dominated by $BB^*$ has energy close to...
FIG. 2: Eigen-energies of $\bar{b}b\bar{d}u$ system (Fig. 1a) for various separations $r$ between static quarks $b$ and $\bar{b}$ are shown by points. The label indicates which two-hadron component dominates each eigenstate. The dot-dashed lines represent related two-hadron energies $E_{n,i}^{\pm}$ when two hadrons do not interact. The eigenstate dominated by $B\bar{B}^*$ (red circles) has energy significantly below $m_B + m_{\bar{B}}$, and shows sizable attraction. Lattice spacing is $a \simeq 0.124$ fm.

Towards masses of $Z_b$ states within certain approximations: Eigen-energies of $b\bar{b}d\bar{u}$ system in Fig. 1a indicate that eigenstate dominated by the $B\bar{B}^*$ has significantly lower energy than $m_B + m_{\bar{B}}$, at small separation $r$ between static $b$ and $\bar{b}$. This suggests a possible existence of exotic hadrons (related to $Z_b$) and peaks in cross-section near $B\bar{B}^*$ threshold. Such physical observables require the study of motion of heavy degrees of freedom based on energies $E_n(r)$ according to Born-Oppenheimer approach. The precise prediction of such observables is not possible at present since lattice eigen-energies are not known for $r < a$. In addition, the accurate study would require coupled-channel treatment of all Fock components through coupled-channel Schrödinger equation, which is a challenging task left for the future (this was recently elaborated in [29] for conventional $bb$ with $I=0$).

We apply two simplifying approximations in order to shed light on the possible existence of $Z_b$ based on energies in Figure 2. The first assumption is that the eigenstate indicated by red circles in Fig. 2 is related exclusively to $B\bar{B}^*$ Fock component and does not contain other Fock components in (1). This is supported by our lattice results to a very good approximation, since this eigenstate couples almost exclusively to $O^{B\bar{B}^*}$ and has much smaller coupling to $O^{\pi\tau}$ and $O^{\bar{B}b_1}$. The normalized overlap of this state to $O^{\pi\tau}\bar{b}_1$ is $1_{3-6} \leq 0.02$ for $r \leq 3$, while overlap to $O^{BB^*}$ is $1_{1,2} \simeq O(1)$. In the reminder we explore physics implications of this eigen-energy $E_{B\bar{B}^*}(r)$.

The energy $E_{B\bar{B}^*}(r)$ represents the total energy without the kinetic energy of heavy degrees of freedom. The difference $V(r) = E_{B\bar{B}^*}(r) - m_B - m_{\bar{B}}$, therefore represents the potential felt by the heavy degrees of freedom, in this case between $B$ and $\bar{B}^*$ mesons. The extracted potential is plotted in Fig. 3. The potential shows sizable attraction for $r = [0.1, 0.4]$ fm and is compatible with zero for $r \geq 0.6$ fm within sizable errors. Lattice study that would probe whether one-pion exchange dominates at large $r$ would need higher accuracy.

The problem is that potential $V(r)$ is not determined from lattice for $r < a$, it might be affected by discretization effects at $r \simeq a$ and the analytic form of $r$-dependence is not known apriori. This brings us to the second simplifying approximation

$$V(r) = V_{reg}(r) + V_{1/r}(r), \quad V_{reg}(r) = -A e^{-(r/d)^p},$$  \hfill (5)

where we assume a certain form of the regular potential $V_{reg}(r)$ that has no singularity at $r \to 0$. The fits of lattice potential for various choices of power $F$ and
range \( r = [1, 4] \) are shown in Fig. 3 (we have verified that fits \( r = [2, 4] \) lead to similar conclusions). The question if potential contains also a singular piece \( 1/r \) can be addressed perturbatively, giving \( V_{1/r}(r) = 0 \) and \( V_{1/r}(r) = \frac{1}{11}[V_0(r) + 8V_b(r)] = \frac{\delta_{bq}}{108s_\pi^2} \frac{a_1}{s_\pi} \) for very small \( r \). This follows from interaction of \( b \) and \( b \) within \( BB^* \), while other pairs among \( bbqq \) are at average distance of the order of \( B \)-meson size and do not lead to singularity at \( r \to 0 \). Results below are based on \( V_{reg} + V_{1/r} \); we have verified that masses and cross-sections based solely on \( V_{reg} \) agree within the errors since \( V_{1/r} \) is suppressed.

The motion of \( B \) and \( B^* \) within the extracted potential \( V(r) \) is analyzed by solving the non-relativistic 3D Schrödinger equation \[-\frac{1}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} + V(r)]u(r) = \] for experimentally measured \( B^* \) meson masses and \( 1/\mu = 1/m_{B^*} + 1/m_{B^*} \). Here \( W = E^{tot} - m_B - m_{B^*} \) is the energy with respect to \( BB^* \) threshold. The \( B \) and \( B^* \) can couple to \( Z_b \) channel with \( J^P = 1^+ \) in partial waves \( l = 0, 2 \). Below we extract (virtual) bound states and scattering rates for \( l = 0 \), while \( l = 2 \) is not discussed since \( V(r) + \frac{l(l+1)}{2\mu r^2} > 0 \) is repulsive for all \( r \).

Wave functions of the Schrödinger equation render the phase shift \( \delta_{bq}(W) \) and \( BB^* \) scattering matrix \( S(W) = e^{2i\delta_{bq}(W)} \). Resonances above threshold do not occur for purely attractive s-wave potentials since there is no barrier to keep the state metastable, while (virtual) bound states below threshold may be present. Bound state (virtual bound state) corresponds to the pole of \( S(W) \) for real \( W < 0 \) and imaginary momenta \( k = i|k| \) \( (k = -i|k|) \) of \( B \) and \( B^* \) in the center of momentum frame.

We find a virtual bound state below threshold and its location is shown by diamonds in Fig. 3; this pole is present when the parameter \( F \) in \( V \) is \( F < 1.9 \). If this pole is close below threshold, it enhances the \( BB^* \) cross-section above threshold. For example, we find a virtual bound state with mass \( M \) slightly below threshold

\[
M - m_B - m_{B^*} = -13 \pm 10 \text{ MeV} , \tag{6}
\]

for the values of parameters \( F = 1.3, A = 1.139(50), d = 1.615(71) \) in \( V \). This state is responsible for a peak in the \( BB^* \) rate \( N_{BB^*} \propto k\sigma \propto \sin^2 \delta_0(W)/k \) above threshold, shown in Fig. 3 for the central value of parameters. The shape of the peak resembles the \( Z_6(10610) \) peak in the \( BB^* \) rate observed by Belle (Fig. 2 of 3).

The significantly attractive \( BB^* \) potential (Fig. 3), and the resulting virtual bound state (diamonds in Fig. 3) could be related to the existence of \( Z_b \) in experiment. The reliable relation between both will be possible only when simplifications employed here will be overcome in the future simulations. We note that \( Z_6(10610) \) was found as a virtual bound state slightly below threshold also by the re-analysis of the experimental data [4] when the coupling to bottomonium light-meson channels was turned off [4] (the position of the pole is only slightly shifted when this small coupling is taken into account).

Surprisingly, the strongly attractive potential \( V(r) \) leads also to a deep bound state at \( M - m_B - m_{B^*} = -411 \pm 20 \text{ MeV} \). Such a state was never reported by experiments. If our approach can be trusted for such deep bound states and if such a bound state exists, it could be searched for in \( Z_b \to \Upsilon(1S)\pi^+ \) decays. The invariant mass distribution observed by Belle is indeed not flat (Fig. 4a of 2) and it would be valuable to explore if some structure becomes significant at better statistics.

The exotic \( Z_b \) resonances were observed only by Belle, so their confirmation by another experiment would be highly welcome. LHCb could try to search for it in inclusive final state \( BB^* \).

**Conclusions:** We presented a lattice QCD study of a channel with quark structure \( b\bar{b}d\bar{u} \), where Belle observed two exotic \( Z_b \) hadrons. We find significantly attractive potential \( V(r) \) between \( B \) and \( B^* \) at small \( r \) when the total spin of the heavy quarks is equal to one. Dynamics of \( BB^* \) system within the extracted \( V(r) \) leads to a virtual bound state, whose mass depends on the parametrization of \( V \). Certain parametrizations give a virtual bound state
slightly below $B\bar{B}$ threshold and a narrow peak in $B\bar{B}^*$ rate just above threshold, resembling $Z_b$ in experiment.

For quantitative comparison to experiment, future lattice studies need to explore how the dynamics of $B\bar{B}^*$ is influenced by the coupling to $\Upsilon\pi$ channels, and by the component where the total spin of the heavy quarks is equal to zero. Derivation of the appropriate analytic form for $V(r)$ would be very valuable.

Acknowledgments: We thank G. Bali, V. Baru, P. Bicudo, N. Brambilla, E. Braaten, M. Karliner, R. Mizuk, A. Peters and M. Wagner for valuable discussions. S.P. acknowledges support by Research Agency ARRS (research core funding No. P1-0035 and No. J1-8137) and DFG grant No. SFB/TRR 55. H.B. acknowledges support from the Scientific and Technological Research Council of Turkey (TUBITAK) BIDEB-2219 Postdoctoral Research Programme.

* sasa.prelovsek@ijs.si

[1] Belle, A. Bondar et al., Phys. Rev. Lett. 108, 122001 (2012), arXiv:1110.2251.
[2] Belle, A. Garmash et al., Phys. Rev. D91, 072003 (2015), arXiv:1403.0992.
[3] Belle, A. Garmash et al., Phys. Rev. Lett. 116, 212001 (2016), arXiv:1512.07419.
[4] Q. Wang et al., Phys. Rev. D98, 074023 (2018), arXiv:1805.07453.
[5] X.-W. Kang, Z.-H. Guo and J. A. Oller, Phys. Rev. D94, 014012 (2016), arXiv:1603.05546.
[6] P. G. Ortega, J. Segovia, D. R. Entem and F. Fernandez, The charged $Z_c$ and $Z_b$ structures in a constituent quark model approach, in 24th European Conference on Few-Body Problems in Physics (EFB24) Surrey, UK, September 2-6, 2019, [1910.06579].
[7] G.-J. Wang et al., Eur. Phys. J. C79, 567 (2019), arXiv:1811.10339.
[8] Y.-C. Yang, Z.-Y. Tan, H.-S. Zong and J. Ping, Few Body Syst. 60, 9 (2019), arXiv:1712.09285.
[9] M. B. Voloshin, Phys. Rev. D96, 094024 (2017), arXiv:1707.00565.
[10] F. Goerke, T. Gutsche, M. A. Ivanov, J. G. Krner and S. Schaefer, Phys. Rev. D78, 054511 (2008), arXiv:0806.4586.
[11] C. Michael, Nucl. Phys. B259, 58 (1985).
[12] M. Luscher and U. Wolff, Nucl. Phys. B339, 222 (1990).
[13] B. Blossier, M. Della Morte, G. von Hippel, T. Mendes and R. Sommer, JHEP 04, 094 (2009), arXiv:0902.1265.
[14] P. Bicudo, M. Cardoso, N. Cardoso and M. Wagner, 1910.04827.
[15] B. A. Kniehl, A. A. Penin, Y. Schroder, V. A. Smirnov and M. Steinhauser, Phys. Lett. B607, 96 (2005), arXiv:hep-ph/0412083.
SUPPLEMENTARY INFORMATION

S1: SYMMETRIES AND OPERATORS

Here we provide more details on the transformation properties of the investigated system in Fig. 1(a) with quantum numbers in Eq. (2). Transformations and quantum numbers are considered on the example of operators $O_1$ and $O_4$ (3). The first line in $O_1$ separates Dirac indices of heavy and light quarks, which simplifies specific transformations.

The $z$-component of the angular momentum $J_z = 0$ is the eigenvalue related to the rotation of the light degrees of freedom around $z$-axes. The light-quark part of $O_1$ is $\bar{q}^b \Gamma_{BA} q^a \propto \bar{q}^b (1 - \gamma_t) \gamma_5 q^a$, which has angular momentum equal to zero. The light degrees of freedom in $O_4$ are represented by the pion with momentum $p \propto e_z$ and a straight gauge link path $U$ between 0 and $r$. Both have $z$-component of the angular momentum equal to zero.

The quantum number $\epsilon = -1$ is related to the reflection of light-degrees of freedom over $yz$ plane, which is a product of rotation $R_{x, \pi}$ by $\pi$ around $x$ and inversion $I$ with respect to the midpoint between 0 and $r$. The light-quark part $\bar{q}^b (1 - \gamma_t) \gamma_5 q^a$ of $O_1$ is invariant under rotations and has $P = -1$, therefore $\epsilon = -1$. The pion with momenta in $z$-direction within $O_4$ transforms as $\pi_{-\epsilon_z} \rightarrow \pi_{-\epsilon_z} I = -\pi_{\epsilon_z}$, while the straight gauge link is invariant under this reflection, so $\epsilon = -1$.

The Dirac structure for the heavy quark part in all operators is $\bar{b} \gamma_5 P_u b$, which ensures $S^b = 1$ and $S^u_b = 0$.

The $C \cdot P = -1$ is related to the reflection of charge-conjugation and inversion with respect to the midpoint between 0 and $r$. Both refer to the transformation of the light-degrees of freedom as well as the transformation of the static colour source ($\psi$). This is most conveniently accomplished by the usual transformation rules $\psi \rightarrow C \bar{\psi}^T$ and $\psi \rightarrow \gamma_5 \psi$ for both $\psi = q$ and $b$, where this operation does not affect the heavy quark spin, while $C = i \gamma_2 \gamma_t$.

The operator $O_1$ has $C \cdot P = -1$ since

$$O_1 = \sum_{a,b} \bar{b}^a(0) \tilde{\Gamma} b^b(r) \tilde{\psi}^a(r) \Gamma q^a(0) \quad \text{(S1)}$$

where $P$ exchanges positions 0 and $r$, $\gamma_t C \tilde{T} C \gamma_5 = \tilde{T}$ for $\tilde{T} = \gamma_5 P_+, \gamma_t C \tilde{T} C \gamma_5 = -\Gamma$ for $\Gamma = P_+ \gamma_5$, and dummy indices $a \leftrightarrow b$ can be exchanged in the last expression. The linear combination $\pi_{\epsilon_z} \rightarrow \pi_{-\epsilon_z} - \pi_{\epsilon_z}$ ensures good $C \cdot P = -1$ for $O_4$.

The second line in operator $O_1$ (3) is obtained via the Fierz rearrangement

$$\tilde{\Gamma} C \tilde{T} \Gamma_{BA} = \frac{1}{16} \sum_{\Gamma, \gamma^2, \Gamma} \text{Tr}[\Gamma^1 \tilde{T}^2 \Gamma^1] C_{\gamma^2 A} \Gamma_{\gamma^2 D} \quad \text{(S2)}$$

and further simplifies since static heavy quarks appear in the combination $P_+ b$ and $\bar{b} P_-$. 

S2: EFFECTIVE ENERGIES AND OVERLAPS

Effective energies $E^{eff}$ of the system in Fig. 1a are shown in Fig. [S1] for separation $r/a = 2$ and all eigenstates $n = 1 \ldots 6$. Effective energies are obtained from correlation matrices $C_{ij}(t)$ via variational approach $C(t) u_n(t) = \lambda_n(t) C(t_0) u_n(t)$, where effective energies are given by the eigenvalues $E_n^{eff}(t) \equiv \lambda_n(t)/\lambda_n(t + 1)$. Reference time $t_0 = 2$ is used and agreement for $t_0 = 3, 4$ is verified. Effective energies render eigen-energies $E_n$ in the plateau region, indicated in the plots.

The overlaps $\langle O_1 | n \rangle$ of each eigenstate $n$ to employed operators $O_1$ (3) are shown in terms of the normalized overlapped $Z_n^i$ in Fig. [S1b]. Here $Z_n^i \equiv \langle O_1 | n \rangle / \max_m \langle O_1 | m \rangle$ is normalized so that its maximal value for given $O_1$ across all eigenstates is equal to one. Overlaps of the eigenstate dominated by $BB^*$ (red circles in Fig. 2) are in Fig. [S2].

S3: POTENTIAL BETWEEN $B$ AND $\bar{B}^*$ FROM LATTICE

The lattice potential $V(r)$ between $B$ and $\bar{B}^*$ from Fig. 3a is tabulated in Table [S1]

| $r/a$ | $V(r)$       |
|-------|--------------|
| 1     | $-0.659 \pm 0.017$ |
| 2     | $-0.341 \pm 0.021$ |
| 3     | $-0.102 \pm 0.025$ |
| 4     | $-0.0150 \pm 0.0157$ |

TABLE S1: Potential $V(r)$ between $B$ and $\bar{B}^*$ extracted from our simulation and plotted in Fig. 3a. Potential $V(r)$ for separations $r/a > 4$ is equal to zero within statistical and systematic errors.

1 If the color of the static source was not transformed under the charge-conjugation, the color-singlet $\bar{b} \gamma_t q^a \bar{q} b^b$ would transform under $C$-conjugation to $\bar{b} C \bar{q} \gamma_5 C \tilde{T} C \bar{q} b^b$, which is not gauge invariant.
FIG. S1: (a) Effective energies $E_{eff}^n$ of the system in Fig. 1a for separation $r/a = 2$ and all eigenstates $n = 1,..,6$. They render eigen-energies $E_n$ in the plateau region. (b) Normalized overlaps $\tilde{Z}_i^n \propto \langle O_i | n \rangle$ of each eigenstate $n$ on the left to six operators $O_{i=1,6}$. Absolute values of overlaps are shown for $r/a = 2$.

FIG. S2: Overlaps $\tilde{Z}_i^n \propto \langle O_i | n \rangle$ of the eigenstate dominated by $B\bar{B}^*$ (red circles in Fig. 2) for separations $r/a = [1,4]$. Absolute value of overlap is shown in logarithmic scale.

S4: POTENTIAL BETWEEN $B$ AND $\bar{B}^*$ AT VERY SMALL SEPARATION $r$

Here we consider the potential between $B$ and $\bar{B}^*$ analytically, where $b$ and $\bar{b}$ are separated by a very small distance $r \ll r_B$, such that $r$ is much smaller than average distance $r_B$ between $b$ and $\bar{q}$ in $B^{(*)}$ meson (i.e. average radius $r_B$ of a static $B^{(*)}$ meson). We address the question whether this potential has a singular form
The singlet and octet contributions cancel in the case of one-gluon exchange, i.e at the order $O(\alpha_s)$. The lowest non-zero contribution can be obtained from the perturbative calculation of both potentials in \[30\] and comes at $O(\alpha_s^2)$ with $\delta a_2 = -189.2$. Employing the value of $\alpha_s \simeq 0.31$ obtained from the fit of the singlet $\bar{b}b$ static potential in our simulation, we arrive at $V_{1/r}(r) \simeq -0.0051/r$.

\section*{S5: Masses of (Virtual) Bound States for Various Fits}

The masses of (virtual) bound states in Fig. 4 of the main article were based on the fits of the lattice potential in the range $r/a = [1, 4]$ and form of potential $V(r) = V_{reg}(r) + V_{1/r}(r)$ in Eq. (5): these masses are shown again in Fig. S3(a) for completeness. The lattice potential at $r/a = 1$ can be prone to lattice discretization errors, therefore we investigate in sensitivity of the results onexcluding this point from the fit. The masses based on the fits in the range $r/a = [2, 4]$ are shown in Fig. S3(b). They also support the presence of a virtual bound state for values of parameter $F < 2$ and a deep bound state $350 - 400$ below threshold, so the results qualitatively agree in both cases.

The part of the potential $V_{1/r}(r)$ that is singular as $r \to 0$ was determined perturbatively \[S5\] for very small separations $r$. It is equal to zero at the one-gluon exchange level and the lowest non-zero contribution comes at the order $O(\alpha_s^2)$. The sensitivity of the results on including or excluding this part of the potential is explored in Fig. S3. The masses based solely on the regular potential $V_{reg}$ in Figs. S3(c,d) agree within errors with masses based on $V_{reg} + V_{1/r}$ in Figs. S3(a,b). This agreement is a consequence of the suppression in $V_{1/r}$.

The task is therefore to determine potential between $b$ and $b$ within a pair of color-singlet $B^{(*)}$ mesons

$$|B\bar{B}^*| = \frac{1}{\sqrt{3}}(\bar{b}q) \frac{1}{\sqrt{3}}(\bar{q}b) = \frac{1}{3} \sum_{a=1,3} \sum_{b=1,3} \bar{b}_a q_a \bar{q}_b b_b.$$  \hspace{1cm} \text{(S3)}$$

The color structure with indices $a$ and $b$ matches with employed operators $O^{B\bar{B}^*}$, while other indices will not be relevant below. In order to determine the potential, $|B\bar{B}^*|$ is expressed in terms of color singlets and octets

$$|B\bar{B}^*| = \frac{1}{3} \{ \frac{1}{\sqrt{3}}(\bar{b}b) (\frac{1}{\sqrt{3}}(\bar{q}q)) + \sum_A (\frac{1}{\sqrt{2}} \bar{b}A_A b)(\frac{1}{\sqrt{2}} \bar{q}A_A q) \}.$$  \hspace{1cm} \text{(S3)}$$

The $\bar{b}b$ singlet within $(B\bar{B}^*|B\bar{B}^*)$ renders singlet potential $V_0(r)$, all eight octets render octet potential $V_8(r)$

$$\langle \frac{1}{\sqrt{3}}(\bar{b}b) \frac{1}{\sqrt{3}}(\bar{q}b) \rangle \to V_0(r) = -\frac{4}{3} \alpha_s \frac{r}{r} \cdot O(\alpha_s^2),$$  \hspace{1cm} \text{(S4)}$$

$$\langle \frac{1}{\sqrt{2}} \bar{b}A_A b \frac{1}{\sqrt{2}} \bar{q}A_A q \rangle \to V_8(r) = \frac{1}{6} \alpha_s \frac{r}{r} \cdot O(\alpha_s^2), \quad A = 1, \ldots, 8,$$

while $\langle \frac{1}{\sqrt{3}}(\bar{q}q) \frac{1}{\sqrt{3}}(\bar{q}b) \rangle \to 1$ and $\langle \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \bar{q}A_A q \rangle \to 1$ are properly normalized to one. The resulting $B\bar{B}^*$ potential at very small $r$ is therefore

$$V_{1/r}(r) = \frac{1}{3} [V_0(r) + 8V_8(r)], \quad V_{1/r}^{O(\alpha_s)}(r) = 0,$$

$$V_{1/r}(r) = \frac{1}{9} \frac{\alpha_s}{3} \frac{r}{r} \cdot \left( \frac{\alpha_s}{4\pi} \right)^2 \delta a_2.$$  \hspace{1cm} \text{(S5)}$$

All other pairs are at average distance of the order of $O(r_B)$, which is finite for $r \to 0$; these pairs do not lead to infinite potential for $r \to 0$ and we therefore omit their contribution to $V_{1/r}$.

$V_{1/r}(r) = \frac{K}{r}$ for $r \to 0$ and determine prefactor $K$, while we omit all sub-leading contributions that are finite at $r \to 0$. Among all pairs of the four quarks $\bar{b}b\bar{q}q$, only interaction between $b$ and $\bar{b}$ at very small $r$ could give potential proportional to $1/r$. All other pairs are at average distance of the order of $O(r_B)$, which is finite for $r \to 0$; these pairs do not lead to infinite potential for $r \to 0$ and we therefore omit their contribution to $V_{1/r}$.

The part of the potential $V_{1/r}(r)$ that is singular as $r \to 0$ was determined perturbatively \[S5\] for very small separations $r$. It is equal to zero at the one-gluon exchange level and the lowest non-zero contribution comes at the order $O(\alpha_s^2)$. The sensitivity of the results on including or excluding this part of the potential is explored in Fig. S3. The masses based solely on the regular potential $V_{reg}$ in Figs. S3(c,d) agree within errors with masses based on $V_{reg} + V_{1/r}$ in Figs. S3(a,b). This agreement is a consequence of the suppression in $V_{1/r}$.
FIG. S3: Mass of the virtual bound state (diamonds) and the bound state (triangles) for various choices of the parameter $F$ in $V(r)$ (5). The plot compares results based on the fit of the lattice potentials in the ranges $r/a = [1, 4]$ (left) and $r/a = [2, 4]$ (right). The results based on the potential $V_{reg.} + V_{1/r}$ (top) and $V_{reg.}$ (bottom) are also compared.