Lattice Prediction for Deeply Bound Doubly Heavy Tetraquarks

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We investigate the possibility of $qq'\bar{b}\,\bar{b}$ tetraquark bound states using $n_f = 2+1$ lattice QCD ensembles with pion masses ≃164, 299, and 415 MeV. Motivated by observations from heavy baryon phenomenology, we consider two lattice interpolating operators, both of which are expected to couple efficiently to tetraquark states: one with a diquark-antidiquark and one with a meson-meson structure. Using nonrelativistic QCD to simulate the bottom quarks, we study the $ud\bar{b}\,\bar{b}$, $\ell s\bar{b}\,\bar{b}$ channels with $\ell = u, d$, and find unambiguous signals for strong-interaction-stable $J^P = 1^+$ tetraquarks. These states are found to lie 189(10) and 98(7) MeV below the corresponding free two-meson thresholds.

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Introduction.—In QCD the attractive nature of the color Coulomb potential for two antiquarks in a 3_c color configuration ensures the existence of strong-interaction-stable $qq'\bar{Q}\,\bar{Q}$ exotics in the limit $m_Q \to \infty$ [1,2]. However, the physical charm and bottom masses are insufficiently heavy for this mechanism to dominate and ensure the existence of doubly charmed or bottom tetraquarks. Whether such exotics exist is thus a dynamical question involving other, generally nonperturbative, effects in these systems.

The spectrum of bottom baryons suggests that doubly bottom tetraquarks should exist and be strong-interaction stable, for the following reasons.

First, the smallness of the observed $B^* - B$, $B_s^* - B_s$, $\Sigma_b^* - \Sigma_b$, and $\Xi_b^* - \Xi_b'$ splittings suggests that m_b is sufficiently large that the heavy-quark limit, in which the heavy-quark spin decouples and a heavy antidiquark behaves like a single heavy quark, is a reasonable approximation for b quarks. The $\Sigma_b - \Lambda_b$ and $\Xi_b' - \Xi_b$ splittings then give a direct experimental measure of the difference in energies between dressed diquarks with light (u, d, s) quark flavor, spin, and color $(F, S_\ell, C) = (\bar{3}_F, 0, \bar{3}_c)$ and $(6_F, 1, \bar{3}_c)$ in the field of a heavy, nearly static color 3_c source. The $\bar{3}_c$ nonstrange $(I = 0, S_\ell = 0)$ and $(I = 1, S_\ell = 1)$ diquarks lie ~145 MeV below, and ~48 MeV above, the corresponding spin average, while the $\bar{3}_c$ us, ds $(F, S_\ell) = (\bar{3}_F, 0)$, and $(6_F, 1)$ diquarks lie ~106 MeV below and ~35 MeV above the corresponding spin average. Following Jaffe [3], we refer to the $(\bar{3}_F, 0, \bar{3}_c)$ and $(6_F, 1, \bar{3}_c)$ configurations as "good diquark" and "bad diquark."

In the doubly heavy $qq'\bar{b}\,\bar{b}$ sector, with q, $q' = u, d, s$ the good qq' diquark configuration is accessible when the two $\bar{b}$'s are in a color 3_c. With no $\bar{b}$-$\bar{b}$ spatial excitation, the $\bar{b}\,\bar{b}$ spin will be $J_h = 1$, producing an associated tetraquark configuration with $J^P = 1^+$. The relevant two-meson thresholds, below which such a tetraquark would be strong-interaction stable, are then BB^* and B_sB^* for the $I = 0$ and $I = 1/2$ members of the $\bar{3}_F$, respectively. The residual spin-dependent interactions in the $J = 0$, 1 mesons making up these threshold states are suppressed by the b mass, the physical thresholds lying 23 and 25 MeV below their corresponding spin-averaged versions. With ~20 MeV of further binding likely from the color Coulomb interaction in the 3_c $\bar{b}\,\bar{b}$ pair, one would expect an $I = 0$, $J^P = 1^+$ $ud\bar{b}\,\bar{b}$ tetraquark bound by considerably more than 100 MeV and a related $J^P = 1^+ \ell s\bar{b}\,\bar{b}$, $\ell = u, d$, isodoublet bound by ~100 MeV, in the limit in which one ignores the nonpointlike nature of the nearly static $\bar{b}\,\bar{b}$ color 3_c source.

Expectations are less clear for the $qq'\bar{c}\,\bar{c}$ tetraquark channels, where spin-dependent light-heavy interactions are less suppressed. Phenomenologically, the $\Sigma_c^* - \Sigma_c$, $\Xi_c^* - \Xi_c'$, $D^* - D$, and $D_s^* - D_s$ splittings are a factor of 3 greater than the corresponding bottom sector splittings, and the $\Sigma_c - \Lambda_c$ and $\Xi_c' - \Xi_c$ splittings, which would reflect purely light-quark spin dependence in the heavy-quark limit, are ~30 MeV less than the corresponding bottom sector splittings. The larger (~140 MeV) $D^* - D$ and $D_s^* - D_s$ splittings also drive the DD^* and D_sD^* strong-decay thresholds farther down below their spin-averaged analogues than is the case in the bottom system, further eating into the potential tetraquark binding generated by the good light diquark configuration. With significantly reduced net spin-dependent attraction, other residual effects will become more important to take into account quantitatively in the double-charm sector.

Many studies in the literature argue for the existence of strong-interaction-stable doubly heavy tetraquarks [1–11], with the majority of these, moreover, identifying the $\bar{3}_F$, $J^P = 1^+$ channel as optimal for binding. The long distance $J^P = 1^+$ DD^* and BB^* interactions, mediated by pseudoscalar exchange and hence constrained by chiral symmetry, are known to be attractive [2,5], with a strength capable of producing weak binding in the BB^* system [2]. Doubly heavy tetraquark channels have also been investigated in a number of lattice studies [6–10]. The simulations all have $m_\pi > 330$ MeV and, with the exception of Ref. [9], treat the heavy quarks in the static limit. All find the strongest attraction in the $I = 0$, $J^P = 1^+$ channel. Evidence of increasing attraction with decreasing light quark mass is also found. References [7,8,10] employ a Born-Oppenheimer approach, fitting static energies as a function of heavy diquark separation, r, to an assumed functional form, $V(r)$, and then solving for the heavy-quark motion using the Schrödinger equation with potential $V(r)$. The most recent of the studies employing $n_f = 2$ ETMC ensembles [10] uses a screened color Coulomb form for $V(r)$ and, extrapolating linearly to physical m_π, obtains an estimated binding of 90^{+43}_{-36} MeV in the $ud\bar{b}\,\bar{b}$ channel. Bound doubly bottom states, and sometimes bound doubly charmed states, were also obtained in calculations employing a range of model-dependent effective quark-quark interactions [1,11]. The effective interactions employed in these studies all produce a good diquark–bad diquark splitting compatible in sign and magnitude with that required for understanding the features of the meson and baryon spectra.

In what follows, we investigate more quantitatively the expectation that a $\bar{3}_F$ of doubly heavy strong-interaction-stable tetraquark states exists via lattice calculations. Since the arguments above suggest that binding will be greatest in the bottom sector and will increase as the light quark mass is decreased, we focus on the $ud\bar{b}\,\bar{b}$ and $\ell s\bar{b}\,\bar{b}$ channels, and employ publicly available $n_f = 2+1$ ensembles with sufficiently low m_π to allow for a controlled chiral extrapolation. The ensembles used have near-physical m_K and $m_\pi \simeq 164$, 299, and 415 MeV. We work at a fixed lattice spacing and use nonrelativistic QCD (NRQCD) for the b quarks. With significant binding expected, a simple, well-adapted $\bar{3}_F$, $J^P = 1^+$ operator choice should suffice to extract the ground state tetraquark signal. In fact, we employ two operators, one having the diquark-antidiquark structure suggested by the discussions above, and another whose flavor-spin-color correlations are those of the two-meson BB^* and B_sB^* threshold states. Including the latter allows us to reduce excited state contamination of the ground state signal at earlier Euclidean times through a 2×2 generalized eigenvalue problem (GEVP) analysis. The results of our analysis bear out the expectations outlined above, producing strong evidence for deeply bound $ud\bar{b}\,\bar{b}$ and $\ell s\bar{b}\,\bar{b}$ states.

Key features that distinguish our calculation from previous lattice explorations are the use of NRQCD, thus avoiding the static approximation for the heavy b quarks, and the use of ensembles with light quarks close to the physical point.

Lattice operators and correlators.—The general form of a Euclidean time, lattice QCD correlation function is (see, e.g., Ref. [12])

$$C_{O_1O_2}(p,t) = \sum_x e^{ipx}\langle O_1(x,t)O_2(0,0)^\dagger\rangle, \\ = \sum_n \langle 0|O_1|n\rangle\langle n|O_2|0\rangle e^{-E_n(p)t}, \tag{1}$$

where the operators (O_i) have the quantum numbers of the continuum state of interest. For the $I(J^P) = \frac{1}{2}(0^-)$, $\frac{1}{2}(1^-)$ $B(5279)$, and $B^*(5325)$ mesons, for example [13],

$$P(x) = \bar{b}_a^\alpha(x)\gamma_5^{\alpha\beta}u_a^\beta(x), \\ V(x) = \bar{b}_a^\alpha(x)\gamma_i^{\alpha\beta}d_a^\beta(x). \tag{2}$$

We are focused on the $\bar{3}_F$, $J^P = 1^+$ $ud\bar{b}\,\bar{b}$ and $\ell s\bar{b}\,\bar{b}$ channels, and we aim to construct lattice interpolating operators having good overlap with the expected tetraquark ground states.

Our first operator has the favorable diquark-antidiquark structure noted above, with $\bar{b}\,\bar{b}$ color 3_c, spin 1, and light quark flavor spin color $(\bar{3}_F, 0, \bar{3}_c)$ [14]:

$$D(x) = [u_a^\alpha(x)]^T(C\gamma_5)^{\alpha\beta}q_b^\beta(x) \\ \times \bar{b}_a^\kappa(x)(C\gamma_i)^{\kappa\rho}[\bar{b}_b^\rho(x)]^T, \tag{3}$$

where $q = d$ or s. Though there can be relative orbital momentum, the ground state should have none, yielding a $J^P = 1^+$ state. In general, $D(x)$ will also couple to any pair of conventional mesons with the same quantum numbers (the lowest lying being BB^* with $L = 0$ for $q = d$ and B_sB^* with $L = 0$ for $q = s$). Combining a pair of heavy-light mesons on the lattice, we are led to consider a meson-meson operator,

$$M(x) = \bar{b}_a^\alpha(x)\gamma_5^{\alpha\beta}u_a^\beta(x)\bar{b}_b^\kappa(x)\gamma_i^{\kappa\rho}d_b^\rho(x) \\ - \bar{b}_a^\alpha(x)\gamma_5^{\alpha\beta}d_a^\beta(x)\bar{b}_b^\kappa(x)\gamma_i^{\kappa\rho}u_b^\rho(x), \tag{4}$$

for the $\bar{3}_F$, $I = 0$ channel, and the analogous operator with B_sB^* structure for the $\bar{3}_F$ isodoublet channel.

To study possible tetraquark binding, we compare the ground state and lowest-lying free two-heavy-light meson state mass sum in the channel of interest. This can be achieved by using the relevant pseudoscalar (P) and vector (V) meson correlators, $C_{PP}(t)$ and $C_{VV}(t)$ of Eq. (2), to compute the binding correlator,

$$G_{O_1O_2}(t) = \frac{C_{O_1O_2}(t)}{C_{PP}(t)C_{VV}(t)}, \tag{5}$$

which, for a channel with a tetraquark ground state with (negative) binding ΔE with respect to its two-meson PV threshold, grows as $e^{-\Delta Et}$ for a large Euclidean t.

GEVP analysis.—The operators [Eqs. (3) and (4)] have the same quantum numbers and hence overlap with the same ground and excited states, though with different relative strengths. We define the matrix of binding

TABLE I. Overview of our ensemble parameters: $am_{\pi,K}$ are from global cosh or sinh fits to a shared mass and common amplitudes over the C_{PP}, $C_{A_tA_t}$, and C_{A_tP} correlators using both wall-local and wall-wall data. Fit ranges were chosen so χ^2/d.o.f. is close to 1. This analysis leads to am_π with uncertainties improved by a factor of ~6 relative to those of Ref. [16]. Throughout, the strange quark is tuned to its physical value in the valence sector with $\kappa_s^{\rm val} = 0.13666$. These configurations use the Iwasaki gauge action [17] with $\beta = 1.9$ and nonperturbative clover coefficient $c_{SW} = 1.715$.

Label	E_H	E_M	E_L
Extent	$32^3 \times 64$	$32^3 \times 64$	$32^3 \times 64$
a^{-1}[GeV] [18]	2.194(10)	2.194(10)	2.194(10)
κ_l	0.13754	0.13770	0.13781
κ_s	0.13640	0.13640	0.13640
am_π	0.18928(36)	0.13618(46)	0.07459(54)
am_K	0.27198(28)	0.25157(30)	0.23288(25)
$m_\pi L$	6.1	4.4	2.4
M_Υ[GeV]	9.528(79)	9.488(71)	9.443(76)
Configurations	400	800	195
Measurements	800	800	3078

correlation functions, including possible operator mixing, by

$$F(t) = \begin{pmatrix} G_{DD}(t) & G_{\rm DM}(t) \\ G_{MD}(t) & G_{MM}(t) \end{pmatrix}. \qquad (6)$$

The variational method can then be used to extract the binding by solving the GEVP,

$$F(t)\nu = \lambda(t)F(t_0)\nu, \qquad (7)$$

with the eigenvectors ν and the binding energy determined directly from the eigenvalues $\lambda(t)$ via

$$\lambda(t) = Ae^{-\Delta E(t-t_0)} = (1+\delta)e^{-\Delta E(t-t_0)}. \qquad (8)$$

From a 2×2 matrix, two eigenvalues can be extracted: one corresponds to the ground state and the other to a mixture of all excited state contaminations.

Numerical setup.—We use $n_f = 2+1$ Wilson-Clover [15] fermion gauge field ensembles generated by the PACS-CS Collaboration [16], with a partially quenched valence strange quark tuned to obtain the physical K mass at the physical point. An overview of the ensembles can be found in Table I. The basic spectrum of Ref. [16] was reproduced in this Letter. In the valence sector, we used Coulomb gauge-fixed wall sources. (The FACG algorithm of Ref. [19] was used to fix to an accuracy of $\Theta < 10^{-14}$.) Sources on multiple time-source positions were inverted to compute light, strange, and bottom quark propagators. (We use a modified deflated SAP solver [20] for the light and strange quarks).

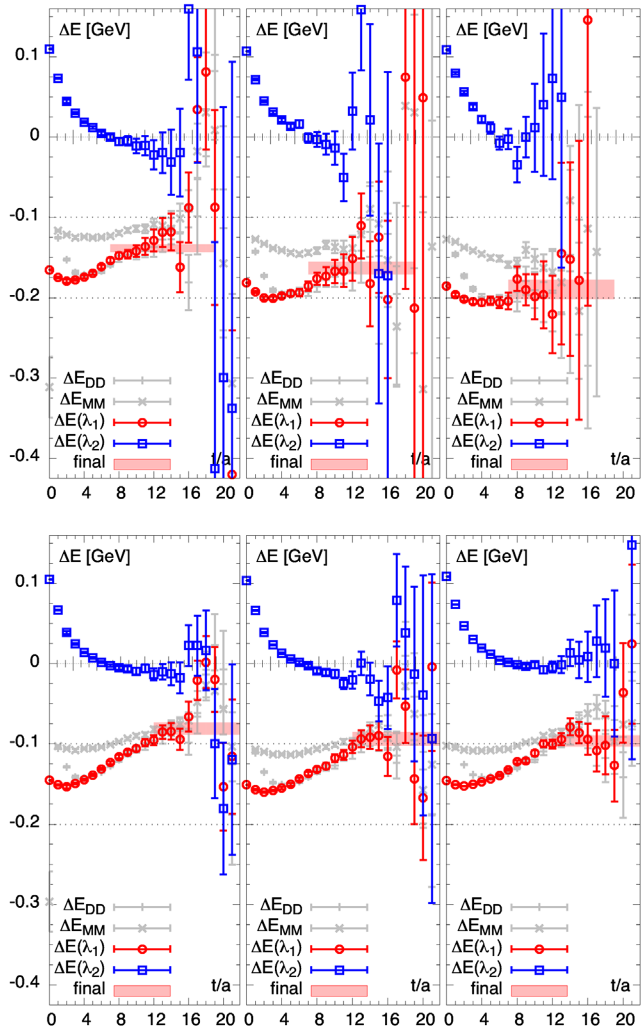

FIG. 1. (Top panel) $ud\bar{b}\,\bar{b}$ and (bottom panel) $\ell s\bar{b}\,\bar{b}$ tetraquark effective binding energies. Red circles (blue squares) represent the bindings relative to the BB^* (B_sB^*) threshold of the first and second GEVP eigenvalues, respectively. Red bands denote the final fit results. Grey dashes and grey crosses indicate the bindings obtained from the corresponding diquark-diquark and meson-meson single-operator analyses. (Left panels) $E_H(m_\pi L \simeq 6.1, m_\pi \simeq 415$ MeV). (Center panels) $E_M(m_\pi L \simeq 4.4, m_\pi \simeq 299$ MeV). (Right panels) $E_L(m_\pi L \simeq 2.4, m_\pi \simeq 164$ MeV).

NRQCD propagators and mass tuning.—We use the NRQCD lattice action [21] to calculate bottom quark propagators. The Hamiltonian is [22]

$$\begin{aligned} H = &-\frac{\Delta^{(2)}}{2M_0} - c_1\frac{(\Delta^{(2)})^2}{8M_0^3} + \frac{c_2}{U_0^4}\frac{ig}{8M_0^2}(\tilde{\boldsymbol{\Delta}}\cdot\tilde{\boldsymbol{E}} - \tilde{\boldsymbol{E}}\cdot\tilde{\boldsymbol{\Delta}}) \\ &- \frac{c_3}{U_0^4}\frac{g}{8M_0^2}\boldsymbol{\sigma}\cdot(\tilde{\boldsymbol{\Delta}}\times\tilde{\boldsymbol{E}} - \tilde{\boldsymbol{E}}\times\tilde{\boldsymbol{\Delta}}) \\ &- \frac{c_4}{U_0^4}\frac{g}{2M_0}\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{B}} + c_5\frac{a^2\Delta^{(4)}}{24M_0} - c_6\frac{a(\Delta^{(2)})^2}{16nM_0^2}, \end{aligned} \qquad (9)$$

with the tadpole-improvement coefficient U_0 set via the fourth root of the plaquette and tree-level values $c_i = 1$. A

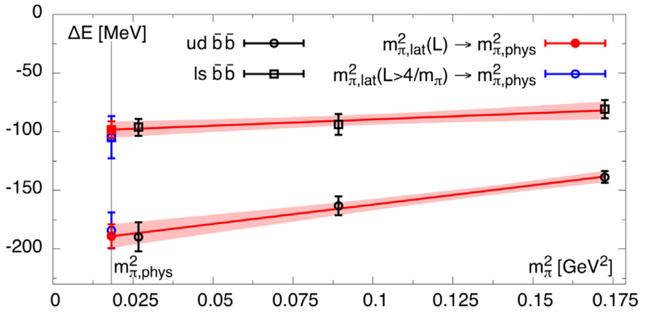

FIG. 2. Chiral extrapolations of the $ud\bar{b}\,\bar{b}$ and $\ell s\bar{b}\,\bar{b}$ binding energies. The red lines and points show the extrapolations using all three ensembles, and the blue points those using E_H and E_M.

tilde denotes tree-level improvement and the c_5, c_6 terms remove the remaining $O(a)$ and $O(a^2)$ errors.

To tune the bottom quark bare mass we calculated the Υ-meson correlation function using local-local hadron correlators at finite momentum. The tuning is implemented via the momentum dispersion relation

$$E(\hat{p}) = M_0 + \frac{1}{2}\frac{\hat{p}^2}{M_{\rm ph}} + \sum_{n>1} O(\hat{p}^{[2n]}), \qquad (10)$$

where we use lattice momenta $\hat{p}_\mu = a\sin(2\pi n_\mu/L_\mu)$. $M_{\rm ph}$ is the physical hadron mass and the values quoted in Table I are from a linear fit in $\hat{p}^2$ to Eq. (10). This setup is known to account for relativistic effects at the few percent level while capturing the relevant heavy-light quark physics [23,24]. (Our own heavy meson and baryon spectrum agrees well with Ref. [24], and a publication is in preparation.)

Numerical results and chiral and volume extrapolations.—Our results for the ground (red) and excited state (blue) binding energies are shown in Fig. 1. For presentational purposes, we show these as log-effective binding energies. For comparison, results obtained from the single-operator diquark-antidiquark (grey dashes) and meson-meson (grey crosses) analyses are also included. The results show that both operators couple well to the ground state. We also see, as t/a increases, the second GEVP eigenvalue approaches the relevant two-meson PV threshold in both channels, strongly supporting an interpretation of the corresponding ground states as genuine tetraquarks. (In addition, we estimated the effect of a possible attractive meson-meson interaction for a hypothetical BB system using the finite volume relations of Ref. [25] and find it to be at the $\Delta E \approx -10$ MeV level for both the ground and threshold energies.)

To estimate the binding energy, we perform a single exponential fit, Eq. (8), to the first eigenvalue $\lambda(t)$ and accept those that satisfy $\chi^2/\text{d.o.f.} \sim 1$. In the case of an increasing exponential in time, which would indicate a state below threshold, the quality of $\chi^2/\text{d.o.f.}$ diminishes as more noise dominated points are added at long distances. We observe this effect and, in order to give conservative estimates, for our final results we choose

TABLE II. Ensemble and extrapolated physical-point (Phys) $ud\bar{b}\,\bar{b}$ and $\ell s\bar{b}\,\bar{b}$ binding energies from fitting all ensembles. Errors for the individual ensembles are statistical. For the extrapolated physical-point entries, the first error is statistical and the second the systematic error estimated as described in the text.

Ensemble	$\Delta E_{ud\bar{b}\,\bar{b}}$ [MeV]	$\Delta E_{\ell s\bar{b}\,\bar{b}}$ [MeV]
E_H	−139(5)	−81(8)
E_M	−163(8)	−94(9)
E_L	−190(12)	−96(7)
Phys	−189(10)(3)	−98(7)(3)

the longest fit range with $\chi^2/\text{d.o.f.} \simeq 1$ in t/a; these are $7 \to 19$ and $12 \to 25$ for the $ud\bar{b}\,\bar{b}$ and $\ell s\bar{b}\,\bar{b}$ channels, respectively.

We use a linear extrapolation in m_π^2 to determine our physical-point tetraquark bindings. (This is the leading order chiral behavior when the strange quark masses on all ensembles have been tuned to the physical value [26], as was done here.) As the ensemble E_L has a small $m_\pi L$, we estimate our finite volume and chiral extrapolation systematic by performing two such extrapolations, one using only E_H and E_M and the other using all three ensembles, taking half the difference of the resulting central values as our systematic error. These extrapolations are shown in Fig. 2, with the filled red symbols giving the physical-point results for the three-ensemble fits, and the open blue symbols the corresponding results for the fits employing only E_H and E_M. The results of both extrapolations are in good agreement, implying that finite volume errors are under control. The individual-ensemble and extrapolated physical-point results are given in Table II. Light quark cutoff effects are at the $O(a^2)$ level and hence are expected to be small, while the NRQCD Hamiltonian in Eq. (9) is $O(a^2)$ improved.

Decay modes suitable for experimental detection.—We discuss briefly decay modes likely to be amenable to experimental searches for the $\bar{3}_F$, $J^P = 1^+$ $qq'\bar{b}\,\bar{b}$ tetraquark candidates identified above.

With a binding of 189 MeV relative to its BB^* strong-interaction-stability threshold, a $ud\bar{b}\,\bar{b}$ tetraquark will lie below BB threshold and hence will also be stable with respect to electromagnetic decays. The same is true of a $\ell s\bar{b}\,\bar{b}$ tetraquark bound by 98 MeV. With both the $ud\bar{b}\,\bar{b}$ and $\ell s\bar{b}\,\bar{b}$ tetraquarks decaying only weakly, the resulting displaced decay vertices should aid in searching for these states experimentally.

Examples of fully reconstructable modes for the weak decay of the $ud\bar{b}\,\bar{b}$ tetraquark are $B^+\bar{D}^0$ and $J/\Psi B^+K^0$, with $\bar{D}^0$ and B^+ being fully reconstructable from $\bar{D}^0 \to K^+\pi^-$, $B^+ \to \bar{D}^0\pi^+$, and K^0 from its $\pi^+\pi^-K_S$ decay. Similarly, $J/\Psi B_sK^+$ and $J/\Psi B^+\phi$ would serve as fully reconstructable modes for the weak decay of the $us\bar{b}\,\bar{b}$ tetraquark, and $B^+D_s^-$, $B_s\bar{D}^0$, $J/\Psi B^0\phi$, and $J/\Psi B_sK^0$ for the $ds\bar{b}\,\bar{b}$ tetraquark.

Conclusions.—We predict the existence of a $\bar{3}_F$ of strong- and electromagnetic-interaction-stable $qq'\bar{b}\,\bar{b}$ tetraquarks with $ud\bar{b}\,\bar{b}$ and $\ell s\bar{b}\,\bar{b}$ member masses 10.415(10) and 10.594(8) GeV, respectively. These states should decay only weakly, with ordinary heavy meson decay products emitted from a displaced vertex.

While the doubly bottom nature of these states may make experimental detection challenging, decay modes with favorable experimental tag possibilities do exist, making searches for these states interesting. Analogous $qq'\bar{c}\,\bar{c}$, $qq'\bar{c}\,\bar{b}$, and $qq'\bar{s}\,\bar{b}$ tetraquarks, if also stable with respect to both strong and electromagnetic decays, would be more easily detectable experimentally. Whether or not such lighter tetraquark states exist is not clear at present, but it is the subject of ongoing investigations, the results of which will be reported in a future publication.

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[13] Greek indices here denote spin, latin indices color, and u, d, s, b quark flavors.

[14] We have used the identity $\epsilon_{eab}\epsilon_{ecd} = \delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc}$; the two terms on the rhs yield identical contributions to the final correlator.

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[27] See https://github.com/RJHudspith/Contractual_Obligations.