Searching for new spin-0 resonances at LHCb

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We study the phenomenology of light spin-0 particles and stress that they can be efficiently searched for at the LHCb experiment in the form of dimuon resonances. Given the large production cross sections in the forward rapidity region together with the efficient triggering and excellent mass resolution, it is argued that LHCb can provide unique sensitivity to such states. We illustrate our proposal using the recent measurement of Upsilon production by LHCb, emphasizing the importance of mixing effects in the bottomonium resonance region. The implications for dimuon decays of spin-0 bottomonium states are also briefly discussed.

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I. INTRODUCTION

The presence of scalar particles is known to be tightly related to the phenomenon of symmetry breaking. The role of scalar degrees of freedom in fundamental theories has therefore been of lasting interest in both experimental and theoretical physics. These efforts have been refocused with the discovery of the Higgs boson, the measured properties of which [1,2] suggest that it provides the dominant source of the breaking of both the electroweak (EW) and flavor sectors, possibly including dark matter. These features provide a strong motivation for continuing searches for new scalar degrees of freedom both at high and low energies.

New scalars coupling to the SM fermions necessarily carry SM flavor quantum numbers or conversely break the SM flavor symmetry. The overall agreement of most measured flavor observables with the corresponding SM predictions, however, severely restricts any new source of flavor breaking. The simplest, but also most restrictive, solution to this problem is to assume that also beyond the SM, the minimal possible flavor breaking consistent with the observed fermion mass and mixing patterns is realized. This assumption often goes under the name of minimal flavor violation (MFV) [6]. It leads to the clear prediction that the couplings between any new neutral spin-0 state and SM matter are predominantly flavor conserving and proportional to the fermion masses.

Even beyond MFV, simply requiring agreement with the existing constraints on new fermion interactions coming from precision low-energy (mostly flavor) experiments typically leads to severe restrictions on the size of flavor-violating and $CP$-violating couplings. In particular, couplings to lighter fermion generations have to be highly suppressed, while the couplings to heavier quarks and leptons are less constrained. One is thus naturally led to consider new spin-0 particles that couple most strongly to the third generation. Similar to the SM Higgs, such resonances tend to decay to the heaviest kinematically allowed final state and can be abundantly produced in hadronic high-energy collisions through loop-induced gluon-gluon fusion, provided they couple to quarks and are sufficiently light.

Despite their potentially large production cross sections, it turns out, however, that new third-generation-philic spin-0 particles may have escaped detection in existing experiments even for moderately large couplings, if they have masses in the ballpark of [10,50] GeV. First of all, given their very small couplings to electrons and EW gauge bosons, such states easily pass most large electron-positron collider (LEP) constraints (see, however, Ref. [7]). Only for masses below about 10 GeV do radiative Upsilon $\Upsilon(n)$ decays [8–10] and rare $B$-meson decays [11–13] provide stringent constraints.

While masses above 50 GeV are already probed by LHC run I data, the existing searches typically become ineffective for softer final states due to trigger requirements and loss of acceptance (counterexamples include Refs. [14,15]). The situation is actually expected to worsen at the higher energies explored at LHC run II and beyond. In the following, we will argue that this represents a great opportunity for the LHCb experiment with its efficient triggering, excellent vertexing and accurate event reconstruction to provide unique probes of...
new spin-0 particles with masses in the range from few GeV to few tens of GeV.

This article is structured as follows. In Sec. II we discuss the relevant spin-0 interactions and study the resulting branching ratios and production cross sections. Our new search strategy for light Higgs-like particles at LHCb is introduced in Sec. III and applied to bottomonium states in Sec. IV. The numerical analyses for the spin-0 cases are performed in Sec. V. We conclude in Sec. VI. Formulas for the partial widths and branching ratios of spin-0 states are collected in the Appendix.

II. GENERALITIES

We choose to work within an effective theory description below the EW breaking scale \((v = 246 \text{ GeV})\), where the relevant Lagrangian is given by

\[
\mathcal{L} = \mathcal{L}_{\text{SM}} + \frac{1}{2}[(\partial P)^2 - m_P^2 P^2 + (\partial S)^2 - m_S^2 S^2] - \sum_f \frac{m_f}{v} (\kappa_P P \gamma_5 f + \kappa_S S \bar{f} f),
\]

(1)

with \(\mathcal{L}_{\text{SM}}\) encoding the SM interactions. One can easily match the above interactions to more complete EW descriptions above the weak scale, such as multi-Higgs models. In writing (1), we have assumed that the new spin-0 particles \(P, S\) couple to all SM fermions \(f\) in a flavor-conserving way and that their interactions conserve \(CP\), which renders the coefficients \(\kappa_P, \kappa_S\) real. As already discussed in the Introduction, both assumptions are phenomenologically well motivated due to the existing stringent constraints on new sources of flavor and \(CP\) violation (cf. Refs. [11,12,16–20]). However, even the addition of small flavor off-diagonal or \(CP\)-violating couplings consistent with current constraints would affect neither our general discussion nor our conclusions. The same applies to possible couplings of the new mediators to the SM Higgs and EW gauge bosons, which, if present, can provide additional constraints on such scenarios. Since these constraints are strongly model dependent, we will not consider them in what follows.

The simplified model (1) is valid as long as the new scalar \(S\) does not mix strongly with the SM Higgs boson and there are no additional light degrees of freedom below the EW scale. In such a case the model dependence associated to the full Higgs sector is encoded in the portal couplings \(\kappa_{P,S}\). The simplest choice of couplings is universal \(\kappa_{P,S} = \kappa_{P,S}\) and realized in singlet scalar extensions of the SM Higgs sector. Within the decoupling limit of the two-Higgs-doublet model type II (THDMII), one has instead \(\kappa_{P,S} = \tan \beta, \kappa_{P,S} = \cot \beta\) with \(\tan \beta\) denoting the ratio of vacuum expectation values of the two Higgs doublets. More generally, the MFV hypothesis allows for

\[
k_{P,S} = \kappa_D, \kappa_{P,S} = \kappa_U \text{ in the quark sector and } k_{P,S} = \kappa_L \text{ for charged leptons.}
\]

In the mass range of interest and under the assumption that the couplings \(\kappa_{P,S}\) are approximately universal, the mediators \(P, S\) decay dominantly to \(b\bar{b}\) (for \(m_{P,S} > 2m_b\)), \(c\bar{c}\) and \(\tau^+\tau^–\). Somewhat suppressed are instead the \(\mu^+\mu^-\) and \(\gamma\gamma\) branching ratios. These features are illustrated in the two panels of Fig. 1. From these plots it is also evident that for \(|\kappa_{P,S}| \lesssim \mathcal{O}(1)\) the new resonances will be very narrow with the total decay widths not exceeding 1 MeV. The shown results are obtained using the formulas given in the Appendix.

The relative suppression of the clean \(\mu^+\mu^-\) and \(\gamma\gamma\) final states, however, turns out to be of no big concern in practice given the sizeable production rates of light spin-0 states at the LHC. From Fig. 2, one sees that the inclusive cross sections at 8 TeV for a scalar or pseudoscalar of \(\mathcal{O}(10 \text{ GeV})\) mass range from a few nb to tens of nb. The depicted next-to-leading order (NLO) QCD results have been obtained with HIGLU [21] and employ NNPDF30_nlo_as_0118_lhcb parton distribution functions (PDFs) [22]. The use of this specific set is motivated by the fact that these PDFs allow for a better description of small-\(x\) physics, because they include
besides the data incorporated in the standard NNPDF30_nlo_as_0118 fit [23] information on prompt charm production at LHCb [24]. The theory uncertainties that are displayed as colored bands in the plots of Fig. 2 include both PDF and scale ambiguities. The former are obtained by calculating the 68% C.L. envelope of all 50 members of the NNPDF30_nlo_as_0118_lhcb set, while the latter are determined by identifying the renormalization and factorization scales \( \mu = \mu_R = \mu_F \) and varying \( \mu \) in the range \( \mu \in [m_{P,S}/2, 2m_{P,S}] \). We find that using NNPDF30_nlo_as_0118_lhcb PDFs instead of the NNPDF30_nlo_as_0118 set leads to a reduction of the total theoretical uncertainties by more than a factor of 2. To assess the size of \( P, S \) production from bottom-quark annihilation, we have employed the NLO corrections implemented in SusHi [25]. For resonance masses in the bottomonium region, we find that \( \sigma(b\bar{b} \to P, S) \ll \sigma(gg \to P, S) \) and therefore neglect mediator production via bottom-quark annihilation in our numerical analysis. In view of this and given that known (approximate) higher-order QCD corrections to \( gg \to P, S \) [26–31] tend to increase the cross sections, we are confident that \( \sigma(pp \to P) > 6.3 \text{ nb} \ (\sigma(pp \to S) > 3.2 \text{ nb}) \) in the mass region of interest. As will become clear in the next section, from these inclusive production rates a non-negligible fraction of events falls into the LHCb acceptance, which covers pseudorapidities of \( \eta \in [2.0, 4.5] \).

From the above discussion and keeping in mind that hadronic final states suffer from huge backgrounds and poor mass reconstruction, while measurements of diphoton final states are challenging at LHCb, it follows that looking for narrow resonances in dimuon decays seems to be the most promising search strategy at LHCb. In the following we will exploit this general idea by recasting the recent \( \Upsilon(n) \) production measurements of LHCb [32] to derive bounds on the new-physics parameters entering (1). While this particular analysis is only sensitive to new dimuon resonances in the mass range \( m_{P,S} \in [8.6, 12.4] \) GeV, extending the reach with future dedicated studies should be possible. Other previous studies of light spin-0 states using dimuon final states include Refs. [9,11–13,16,17,19,33–35].

### III. Searching for Peaks in the Dimuon Spectrum Close to \( \Upsilon(n) \)

Our discussion is based on the dimuon invariant mass spectrum at \( \sqrt{s} = 8 \) TeV supplied as additional material and also presented in Fig. 1 (right) of the LHCb publication [32]. Using MadGraph5_aMC@NLO [36] generated signal events for spin-0 resonances \( \phi \), matched and showered with PYTHIA 6 [37], we first compute the LHCb acceptance \( A \) based on the cuts \( \eta \in [2.0, 4.5] \) and \( p_T < 30 \) GeV that define the fiducial volume of the measurement. We obtain

\[
A = 0.23,
\]

with negligible dependence on the \( \phi \) mass within the experimental window \( m_\phi \in [8.6, 12.4] \) GeV and its parity. However, the available dimuon invariant mass spectrum data points correspond to a more restrictive kinematical region (i.e. \( \eta \in [3.0, 3.5] \) and \( p_T \in [3.0, 4.0] \) GeV), and the final acceptance \( A_f \) does exhibit a mild dependence on \( m_\phi \). To cross-check our results we have estimated the relative \( \Upsilon(n) \) acceptances \( A_f/A \) by comparing the fitted \( \Upsilon(n) \) event yields in the dimuon spectrum to the corresponding measured fiducial cross sections. We find that the relative acceptances of our generated signal and the LHCb \( \Upsilon(n) \) production are similar when setting the \( \phi \) mass equal to that of \( \Upsilon(n) \). We also considered the LHCb mass resolution and its dependence on \( m_\phi \) by linearly interpolating/extrapolating the widths of the fitted \( \Upsilon(n) \) resonance shapes to higher and lower dimuon invariant masses. These validations give
us confidence that we understand the relative acceptances $A_{\phi}/A$ sufficiently well.

In order to constrain possible new physics signals, we then refit the LHCb data while injecting an additional $\phi$ resonance of a given mass, letting the normalizations of the existing $\Upsilon(n)$ peaks vary freely but keeping their positions fixed. Varying also the normalization of the nonresonant background and performing a $\chi^2$ fit of the full spectrum, we extract the 95% C.L. bounds on the fiducial production cross section times dimuon branching ratio of an additional spin-0 resonance from a recast of the recent LHCb measurement of $\Upsilon$ production. The positions of the physical $\Upsilon(n)$ $(n = 1, 2, 3)$ masses are marked with black dashed lines. Consult the text for further details.

IV. BOUNDS ON DIMUON BRANCHING RATIO OF BOTTOMONIUM STATES

A simple but interesting application of the search strategy introduced in the last section is the derivation of upper limits on the dimuon branching ratios of the pseudoscalar $\eta_b(n)$ and scalar $\chi_b(n)$ bottomonium states. Let us illustrate this in the following.

According to the nonrelativistic QCD (NRQCD) factorization approach [38], the prompt $\eta_b(n)$ production cross section in $pp$ collisions can be written as a convolution of the PDFs $f_{i/j}(x_{1,2})$ with the partonic cross sections $\hat{\sigma}(ij \rightarrow \eta_b(n))$. The partonic cross section factorizes further into perturbative coefficients that encode the production of a $b\bar{b}$ state and nonperturbative matrix elements $\langle \mathcal{O}^{\eta_b(n)} \rangle$ that describe the subsequent hadronization of the $b\bar{b}$ pair into the observable $\eta_b(n)$ states. The matrix elements themselves can be expanded in powers of the relative velocity $v_b^2 = 0.1$ of the $b$ quarks in the bottomonium system.

In fact, the production of $\eta_b(n)$ states is particularly simple, because color-octet Fock states such as $b\bar{b}_8(1S_0), b\bar{b}_8(1S_1)$ and $b\bar{b}_8(1P_1)$ are velocity suppressed compared to the color-singlet $S$-wave contribution $b\bar{b}_1(1S_0)$ [38]. The $b\bar{b}_1(1S_0)$ contribution hence fully dominates $\eta_b(n)$ production [39], and as a result the leading order (LO) gluon-gluon fusion cross sections are given by the following simple expression:

$$\hat{\sigma}(gg \rightarrow \eta_b(n)) = \frac{\pi^3 a_s^2}{36 \alpha_s^2} \delta(1 - 4m_b^2/s) \times \langle 0|\mathcal{O}^{\eta_b(n)}_1(1S_0)|0 \rangle.$$  (3)

Here the strong coupling constant $\alpha_s$ is understood to be evaluated at a scale $\mu_F = 2m_b$ with $m_b \approx 4.75$ GeV the bottom pole mass, while $s$ denotes the partonic center of mass energy. The color-singlet vacuum matrix elements are related to the $S$-wave radial wave functions at the origin via

$$\langle 0|\mathcal{O}^{\eta_b(n)}_1(1S_0)|0 \rangle = \frac{3}{2\pi} |R_{\eta_b(n)}(0)|^2,$$  (4)

and the latter quantities can be extracted from the $\Upsilon(n)$ leptonic decay widths (see for instance Ref. [40]) that are measured accurately [41]. We collect the $|R_{\eta_b(n)}(0)|$ values that are used in our numerical analysis in Table I. Other determinations coming for example from potential models [42] agree with our extractions within uncertainties.

NLO QCD corrections to $\eta_b(n)$ hadroproduction have been calculated in Ref. [43] and include virtual corrections to the $gg \rightarrow b\bar{b}_1(1S_0)$ channel as well as real processes, such as $gg \rightarrow b\bar{b}_1(1S_0)g$ or $gg \rightarrow b\bar{b}_1(1S_0)q$. Employing again NNPDF30_nlo_as_0118_lhcb PDFs, we obtain the following $\hat{\sigma}(\alpha_s^2)$ prediction for the inclusive $\eta_b(n)$ production cross sections,

| $m_{\eta_b(n)}$ | $|R_{\eta_b(n)}(0)|$ | $m_{\chi_b(n)}$ | $|R_{\chi_b(n)}(0)|$ |
|----------------|----------------------|----------------|---------------------|
| $n = 1$        | 9.4                  | 2.71 ± 0.07    | 9.86               |
| $n = 2$        | 10.0                 | 1.92 ± 0.11    | 10.23              |
| $n = 3$        | 10.3                 | 1.66 ± 0.11    | 10.51              |
| $n = 4$        | 10.6                 | 1.43 ± 0.09    | 10.31              |
| $n = 5$        | 10.85                | 1.42 ± 0.53    | 10.56              |
| $n = 6$        | 11.0                 | 0.91 ± 0.17    | 10.70              |
\[ \sigma(pp \to \eta_b(n)) = \frac{(391^{+174}_{-168})|R_{\eta_b(n)}(0)|^2 \text{nb}}{\text{GeV}^2}, \quad (5) \]

for 8 TeV pp collisions. The uncertainties quoted above include both the intrinsic PDF error as well as scale variations \( \mu \in [m_b, 4m_b] \) with \( \mu = \mu_F = \mu_R \). These two types of errors are both asymmetric and similar in size.

Equipped with the production rates (5) and having derived both the LHCb acceptance (2) and the 95\% C.L. limit on the dimuon signal strength in the last section, it is now straightforward to find upper bounds on the \( \eta_b(n) \to \mu^+\mu^- \) branching ratios. In the case of the lightest pseudoscalar bottomonium state, we find for instance

\[
\text{Br}(\eta_b(1) \to \mu^+\mu^-) < \frac{38.4 \text{ pb}}{\sigma(pp \to \eta_b(1))A} = 1.9 \times 10^{-4}. \quad (6)
\]

This limit has been obtained by applying the worst-case method [44], taking 882 nb as the lowest possible pp \( \to \eta_b(1) \) cross section. If the uncertainty in (5) and the error on \( |R_{\eta_b(1)}(0)| \) as reported in Table I are combined in quadrature, this lower bound can be interpreted as a theoretical 95\% C.L. limit. Notice that, even with such a conservative treatment of uncertainties, our limit (6) is stronger by almost a factor of 50 than the 90\% C.L. bound of \( \text{Br}(\eta_b(1) \to \mu^+\mu^-) < 9 \times 10^{-3} \) quoted by the Particle Data Group (PDG) [41]. For the higher pseudoscalar bottomonium states \( \eta_b(2), \eta_b(3), \eta_b(4) \) and \( \eta_b(6) \), our approach leads to worst-case upper bounds on the dimuon branching ratios in the range of \([0.8, 7.3] \times 10^{-4}\). No limits on these branching fractions are provided by the PDG. In the case of \( \eta_b(5) \), on the other hand, the large uncertainty on \( |R_{\eta_b(5)}(0)| \) when extracted from \( \Upsilon(5) \) data, does not allow us to set a meaningful bound.

For the further discussion, we also need predictions for the production cross sections of the bottomonium scalar states \( \chi_b(n) \). Unlike in the case of \( \eta_b(n) \), two Fock states, namely \( bb_1(3P_0) \) and \( bb_b(3S_1) \), contribute to \( \chi_b(n) \) hadroproduction at the same order in the velocity expansion of NRQCD [38]. The color-octet configuration can, however, be produced at \( \mathcal{O}(a_s^2) \) only via \( q\bar{q} \to bb_1(3P_0) \), while in the case of the color singlet the process \( gg \to bb_b(3S_1) \) is possible. Given the high gluon luminosities at the LHC, LO \( \chi_b(n) \) production is hence described to very high accuracy by

\[
\delta(gg \to \chi_b(n)) = \frac{\alpha_s^3}{4\pi^3} \left( 1 - \frac{4m_b^2}{\delta} \right) |\mathcal{O}_{1}(^3P_0)|^2, \quad (7)
\]

with

\[
0|\mathcal{O}_{1}(^3P_0)|^2 = \frac{9}{2\pi} |R_{\chi_b(n)}'(0)|^2. \quad (8)
\]

The derivatives of the \( P \)-wave radial wave functions at the origin \( |R_{\chi_b(n)}'(0)| \) cannot be extracted from experiment, and one thus has to rely on theory to obtain their values. As estimates of the derivatives of the radial wave functions, we take the mean values from the four potential-model calculations presented in Ref. [42]. The numerical values that we employ in our work are tabulated in Table I. The uncertainties given in this table are the standard deviations that derive from the results of the four different potential-model computations.

Like in the case of the \( \eta_b(n) \) states, \( \mathcal{O}(a_s^3) \) corrections to prompt \( pp \to \chi_b(n) \) production are important and have been calculated [43]. Adopting the same methodology that led to (5), we obtain at 8 TeV the NLO result

\[
\sigma(pp \to \chi_b(n)) = \langle 504^{+417}_{-169} \rangle |R_{\chi_b(n)}'(0)|^2 \frac{\text{nb}}{\text{GeV}^2}, \quad (9)
\]

Notice that, as a result of the sizeable \( gg \to bb_1(3P_0) \) contribution which first contributes to \( \chi_b(n) \) hadroproduction at \( \mathcal{O}(a_s^2) \), the uncertainties plaguing (9) are more than twice as large as those entering (5). The above prompt production cross sections can again be translated into lower limits on the \( \chi_b(n) \) dimuon branching ratios. At the 95\% C.L., we obtain \( \text{Br}(\chi_b(n) \to \mu^+\mu^-) \) values in the range of \([1.3, 4.0] \times 10^{-5}\).

The bounds on the dimuon branching ratios that we have derived should be compared to the corresponding SM expectations. Using the formulas given in the Appendix, we obtain

\[
\text{Br}(\eta_b(1) \to \mu^+\mu^-) \approx \text{Br}(\eta_b(1) \to Z^* \to \mu^+\mu^-) = 2 \times 10^{-10} \quad \text{and} \quad \text{Br}(\chi_b(1) \to \mu^+\mu^-) = \text{Br}(\chi_b(1) \to \gamma^* \gamma^* \to \mu^+\mu^-) \approx 7 \times 10^{-11}.
\]

Similar results also hold for all other spin-0 bottomonium states with masses below the open bottom threshold. Our limits are thus around 6 orders of magnitude above the SM expectations.

V. BOUNDS ON NEW SPIN-0 DIMUON RESONANCES

At this point, we have collected all ingredients necessary to interpret the bounds derived in Sec. III in terms of new spin-0 states described by (1) or more specific models like the THDMII. In doing so we need to consider nonperturbative effects due to the presence of bottomonium resonances and the \( b\bar{b} \) threshold. In particular, close to the \( b\bar{b} \) threshold a perturbative description of the production and the decay of the new resonances breaks down. In this region we can, however, approximate the \( b\bar{b} \) contributions to the \( P, S \) widths by a sum over exclusive states interpolated to the continuum sufficiently above threshold [45,46]. Like these analyses, we also assume that the dominant contributions to production and the total width arise from the mixing of the new spin-0 mediators with bottomonium states. In particular, \( P \) will mix with the six \( \eta_b(n) \) states, while \( S \) will mix with the three \( \chi_b(n) \) resonances. Such mixings can effectively be described through off-diagonal contributions \( \delta m_{\eta_b}^2 \) to the pseudoscalar mass matrix squared.
and its analog $M^2_{\eta_b}$ in the scalar case. The masses of the $\eta_b(n) (\chi_b(n))$ states are denoted by $m_{\eta_b(n)} (m_{\chi_b(n)})$, and their numerical values are collected in Table I. The total decay widths $\Gamma_{\eta_b(n)} (\Gamma_{\chi_b(n)})$ of the unmixsed pseudoscalar (scalar) bottomonium states are calculated using the formalism employed in Refs. [45,46]. The relevant expressions are given in the Appendix. The formulas needed to predict the total decay widths $\Gamma_{P;S}$ of the new spin-0 resonances can also be found there.

The off-diagonal entries appearing in (10) can be computed using NRQCD [38]. To zeroth order in $a_s$ and $v_4$, one recovers the nonrelativistic potential model results (see for instance Ref. [45])

\[
\delta m^2_{\eta_b(n)} = \kappa^b \sqrt{\frac{3}{4\pi \eta}} m^3_{\eta_b(n)} |R_{\eta_b(n)}(0)|, \\
\delta m^2_{\chi_b(n)} = \kappa^b \sqrt{\frac{27}{8\pi \Gamma} m_{\chi_b(n)} |R'_{\chi_b(n)}(0)|}.
\]

We identify the physical $P$, $S$ states with the ones containing the largest $P$, $S$ admixture. Their total decay widths can be read off directly from the imaginary parts of the mass matrix squared (10) after diagonalization. The small mass-shift effects [45] needed to avoid level crossing when the $P$, $S$ mass (before mixing) is close to any of the considered bottomonium states are, on the other hand, neglected in our analysis.

The mass mixing has the most significant effect on the couplings of the spin-0 mediators to gluons modifying both the production and the total decay width of the physical (i.e. mixed) $P$, $S$ states. The associated interference in production is affected by the strong phase present in the $gg \to P$, $S$ amplitudes due to intermediate on-shell charm and bottom quarks. Numerically more important than the strong phases are the signs of the couplings $\kappa^{b,h} (\kappa^{b,h})$ relative to $R_{\eta_b(n)} (R'_{\chi_b(n)})$, since these signs determine the interference pattern between the new resonances $P$, $S$ and the QCD spin-0 bound states. For instance, close to the bottomonium resonances, $P$, $S$ production can be significantly enhanced as an effect of mixing. At the same time, however, the decay mode $P$, $S \to gg$ then tends to dominate the total width of the new state, which leads to a further suppression of its dimuon branching ratio. In an accurate calculation, both effects need to be taken into account. Following the discussion in Sec. IV, bottomonium contributions to the dimuon partial widths of the physical $P$, $S$ states are numerically insignificant and can be ignored.

Before presenting our numerical results, we finally note that, since the mixing contributions (11) are proportional to $\kappa^{b,h}$, their impact on the phenomenology of the $P$, $S$ states diminishes (and the effects become more localized to the bottomonium thresholds) as the bounds on the couplings in the simplified model (1) become stronger. Conversely, it turns out that for $\kappa^{b,h} \gtrsim \sqrt{4\pi}$ the large mixings and resulting total $P$, $S$ decay widths start making the identification of physical $P$, $S$ resonances ambiguous as simultaneous mixing with several bottomonium states becomes important. To avoid this issue, we restrict our analysis to the parameter region $\kappa^{b,h} \lesssim \sqrt{4\pi}$.

In Fig. 4 we present the limits on the magnitudes of the universal couplings $\kappa_{P,S} = \kappa^{b,h}$ by employing the 95% C.L. bounds on the dimuon LHCb signal strength derived in Sec. III. The shown exclusions are based on the conservative lower bounds of our cross section calculations shown in Fig. 2 and given in (5) and (9). For comparison, predictions with (red and blue curves) and without (black dashed curves) mixing effects are presented. In the case of mixing, we consider both relative signs of the couplings $\kappa_{P,S}$ to illustrate the associated model dependence. The red (blue) curves correspond to the case where the sign of $\kappa_{P,S}$ is such that the interference in the physical $P$, $S \to gg$ destructive (constructive) for $m_{P,S} < m_{\eta_b(n)}$. From the panels it is evident that, while mixing effects play a particular important role in the pseudoscalar case, due to the large number of QCD resonances and the more pronounced mass mixing $\delta m^2_{\eta_b(n)}$, the obtained bounds are also changed in the scalar case as a result of $\delta m^2_{\chi_b(n)} \neq 0$.

In addition, effects associated to $P \to B^+ \bar{B}^-$ [[see (A25)] are phenomenologically important, since they strengthen the limits on $|\kappa_P|$ visibly for $m_P \in [11,12.4]$ GeV. In the scalar case such effects are instead of minor importance. One finally notices that our proposal allows us to set the first relevant limits of $O(1)$ on the coupling strengths $|\kappa_{P,S}|$ for $m_{P,S} \in [8.6, 11.5]$ GeV. This mass range has so far not been covered by other analyses such as the CMS dimuon search [14], which provides the strongest constraints on $|\kappa_{P,S}|$ for $m_{P,S} \in [5.5, 8.6]$ GeV and $m_{P,S} \in [11.5, 14]$ GeV.
The recent LHCb precision measurement of $\Upsilon(n)$ production thus enables one to close a gap in parameter space.

VI. DISCUSSION AND OUTLOOK

The generic bounds on new light spin-0 states presented in the previous section can be easily interpreted within ultraviolet complete new physics models such as THDM scenarios or the next-to-minimal supersymmetric SM. As an example, we show in Fig. 5 the limits on $\tan\beta$ in the decoupling limit of the THDMII for pseudoscalar masses $m_A$ close to 10 GeV following from our recast (blue curve), the CMS dimuon search [14] (green curve) and the BABAR 90% C.L. limit on radiative $\Upsilon(1)$ decays in the dimuon and ditau channels, respectively. The bound on $\tan\beta$ arising from perturbativity is also shown (black dashed line). All shaded regions correspond to excluded parameter space. For further details see the main text.

From the figure, one observes that the existing analyses of dimuon and ditau final states provide stringent constraints on the THDMII in almost the entire low-$m_A$ mass range, with our recast of the recent LHCb $\Upsilon(n)$ production measurement furnishing the dominant restriction for $m_A \in [8.6, 11]$ GeV. Only the masses $m_A \in [11, 11.5]$ GeV remain unexplored, since mixing effects turn out to be particularly important in this region. We finally recall that the LHCb data used in our fit correspond to only 3% of all recorded dimuon events. Consequently, a dedicated LHCb analysis of the full run I data set is expected to improve the limits derived here considerably, possibly allowing us to surpass the existing CMS constraints for $m_A > 11.5$ GeV.

While we have focused in our work on the experimentally cleanest signature, namely dimuons, light spin-0 resonances could also be searched for in other final states like $\tau^+\tau^-$, $c\bar{c}$ or $b\bar{b}$. All these modes do benefit from larger branching ratios (see Fig. 1) but compared to $\mu^+\mu^-$ do suffer from much more challenging reconstruction and considerably larger backgrounds. The $P, S \to \tau^+\tau^-$ decay in particular seems less promising, because the visible charged particles in the decay are a bad proxy for the total momentum of the taus, with most of the energy typically being carried away by the neutrinos. The resulting invariant mass distribution thus has no pronounced peak for $m_{P, S} \lesssim 15$ GeV. In this respect, LHCb searches for resonances in the exclusive invariant mass spectra of heavy flavored hadrons, such as $D^+D^-$ or $B^+B^-$, may have more potential. A dedicated study of the corresponding phenomenology, while beyond the scope of this work, might hence turn out to be a fruitful exercise.
\[
\Gamma(S \rightarrow gg) = \frac{\alpha_s^2 m_S^4}{32\pi^2 v^2} \sum_q \kappa_q^2 (S(\tau_q^f) + \Delta_{q/S}^f)^2, \quad (A8)
\]

\[
\Gamma(S \rightarrow \gamma\gamma) = \frac{\alpha^2 m_S^3}{64\pi^3 v^2} \left(1 - \frac{m^2}{m_S^2}\right)^3 \left|\sum_f \kappa_f^2 d_f \frac{Q_f^2}{Q_f^2 - \frac{1}{4} m^2} \right|^2, \quad (A9)
\]

\[
\Gamma(S \rightarrow \gamma Z) = \frac{\alpha^2 m_S^3}{32\pi^3 v^2} \left(1 - \frac{m^2}{m_S^2}\right)^3 \left|\sum_f \kappa_f^2 d_f Q_f \right| \left(1 - \frac{2 Q_f s_w^2}{s_w c_w} I_{\gamma Z} \right)^2. \quad (A10)
\]

The relevant loop functions take the form

\[
\mathcal{P}(\tau) = \frac{\tau \arctan^2 \left(\frac{1}{\sqrt{\tau - 1}}\right)}{\sqrt{\tau - 1}}, \quad (A11)
\]

\[
S(\tau) = \tau + (1 - \tau) \mathcal{P}(\tau), \quad (A12)
\]

\[
T(\tau) = \sqrt{\frac{\tau - 1}{\tau}}, \quad (A13)
\]

\[
I(\tau_i, \tau_j) = \frac{\tau_i \tau_j}{2(\tau_i - \tau_j)} \left[\mathcal{P}(\tau_i) - \mathcal{P}(\tau_j)\right], \quad (A14)
\]

\[
J(\tau_i, \tau_j) = \frac{\tau_i \tau_j}{2(\tau_i - \tau_j)^2} \left[\mathcal{P}(\tau_i) - \mathcal{P}(\tau_j)\right] + \frac{\tau_i \tau_j^2}{(\tau_i - \tau_j)^2} \left[T(\tau_i) - T(\tau_j)\right]. \quad (A15)
\]

The perturbative QCD corrections to the partial widths into quark pairs that we include in our analysis are (cf. Ref. [45])

\[
\Delta^q_S = \frac{4\alpha_s}{3\pi} \left(\frac{Q(\beta_q/S)}{\beta_q/S}\right) = \frac{19 + 2\beta_q^2 + 3\beta_q^4}{16\beta_q^2} \ln x_{\beta_q/S} + \frac{21 - 3\beta_q^2}{8}, \quad (A16)
\]

\[
\Delta^q_S = \frac{4\alpha_s}{3\pi} \left(\frac{Q(\beta_q/S)}{\beta_q/S}\right) = \frac{3 + 34\beta_q^2 - 13\beta_q^4}{16\beta_q^2} \ln x_{\beta_q/S} - \frac{3 - 21\beta_q^2}{8}, \quad (A17)
\]

where we have introduced the abbreviation \(x_{\beta_q/S} = (1 - \beta_{i/j})/(1 + \beta_{i/j})\) and the function \(Q(\beta)\) takes the form.
with \( \text{Li}_2(z) \) the usual dilogarithm.

The QCD corrections to the digluon partial widths can be written as (\( \phi = P, S \))

\[
\begin{align*}
\mathcal{G}_P(y) &= \frac{y}{(1-y)^2} \left[ 48 H(1, 0, -1, 0; y) + 4 \ln(1-y) \ln^2 y - 24 \zeta_2 \text{Li}_2(y) - 24 \zeta_2 \ln(1-y) \ln y - 72 \zeta_3 \ln(1-y) \\
- \frac{220}{3} \text{Li}_3(y) - \frac{128}{3} \text{Li}_3(-y) + 68 \text{Li}_2(y) \ln y + \frac{64}{3} \text{Li}_2(-y) \ln y + \frac{94}{3} \ln(1-y) \ln^2 y \\
- \frac{16}{3} \zeta_2 \ln y + \frac{124}{3} \zeta_3 + 3 \ln^2 y - \frac{24 y (5 + 7 y^2)}{(1-y)^3 (1+y)} \text{Li}_4(y) - \frac{24 y (5 + 11 y^2)}{(1-y)^3 (1+y)} \text{Li}_4(-y) \\
+ \frac{8 y (23 + 41 y^2)}{3 (1-y)^3 (1+y)} \text{Li}_3(y) + \text{Li}_3(-y) \ln y - \frac{4 y (5 + 23 y^2)}{3 (1-y)^3 (1+y)} \text{Li}_2(y) \ln^2 y \\
- \frac{32 y (1 + y^2)}{3 (1-y)^3 (1+y)} \text{Li}_2(-y) \ln^2 y + \frac{y (5 - 13 y^2)}{36 (1-y)^3 (1+y)} \ln^4 y + \frac{4 (1 - 17 y^2)}{3 (1-y)^3 (1+y)} \zeta_2 \ln^2 y \\
+ \frac{4 y (11 - 43 y^2)}{3 (1-y)^3 (1+y)} \zeta_3 \ln y + \frac{24 y (1 - 3 y^2)}{(1-y)^3 (1+y)} \zeta_4 + \frac{2 (2 + 11 y)}{3 (1-y)^3} \ln^3 y, \tag{A20}
\end{align*}
\]

\[
\begin{align*}
\mathcal{G}_S(y) &= \frac{y (1+y)^2}{(1-y)^4} \left[ 72 H(1, 0, -1, 0; y) + 6 \ln(1-y) \ln^3 y - 36 \zeta_2 \text{Li}_2(y) - 36 \zeta_2 \ln(1-y) \ln y - 108 \zeta_3 \ln(1-y) \\
- 64 \text{Li}_3(-y) + 32 \text{Li}_2(-y) \ln y - 8 \zeta_2 \ln y - \frac{36 y (5 + 5 y + 11 y^2 + 11 y^3)}{(1-y)^5} \text{Li}_4(-y) \\
- \frac{36 y (5 + 5 y + 7 y^2 + 7 y^3)}{(1-y)^5} \text{Li}_4(y) + \frac{4 y (1+y) (23 + 41 y^2)}{(1-y)^5} [\text{Li}_3(y) + \text{Li}_3(-y)] \ln y, \\
- \frac{16 y (1+y + y^2 + y^3)}{(1-y)^5} \text{Li}_2(-y) \ln^2 y - \frac{2 y (5 + 5 y + 23 y^2 + 23 y^3)}{(1-y)^5} \text{Li}_2(y) \ln^2 y \\
+ \frac{y (5 + 5 y - 13 y^2 - 13 y^3)}{24 (1-y)^3} \ln^4 y + \frac{y (1+y - 17 y^2 - 17 y^3)}{(1-y)^5} \zeta_2 \ln^2 y \\
+ \frac{y (11 + 11 y - 43 y^2 - 43 y^3)}{(1-y)^5} \zeta_3 \ln y + \frac{36 y (1+y - 3 y^2 - 3 y^3)}{(1-y)^5} \zeta_4 - \frac{2 y (55 + 82 y + 55 y^2)}{(1-y)^4} \text{Li}_3(y) \\
+ \frac{2 y (51 + 74 y + 51 y^2)}{(1-y)^4} \text{Li}_2(y) \ln y + \frac{y (47 + 66 y + 47 y^2)}{(1-y)^4} \ln(1-y) \ln^2 y \\
+ \frac{y (6 + 59 y + 58 y^2 + 33 y^3)}{3 (1-y)^5} \ln^3 y + \frac{2 y (31 + 34 y + 31 y^2)}{(1-y)^4} \zeta_3 + \frac{3 y (3 + 22 y + 3 y^2)}{2 (1-y)^4} \ln^2 y \\
- \frac{24 y (1+y)}{(1-y)^3} \ln y - \frac{94 y}{(1-y)^5}. \tag{A21}
\end{align*}
\]

Here \( H(1, 0, -1, 0; y) \) is a harmonic polylogarithm of weight 4 with two indices different from zero, which we evaluate numerically with the help of the program HiPL [48,49]. The polylogarithm of order 3 (4) is denoted by \( \text{Li}_3(z) (\text{Li}_4(z)) \), while \( \zeta_2 = \pi^2/6, \zeta_3 = 1.20206 \) and \( \zeta_4 = \pi^4/90 \) are the relevant Riemann’s zeta values. Finally, the functions multiplying the logarithms \( \ln \mu_R^2/m_q^2 \) in (A19) are given by \( \mathcal{M}_P(\tau) = 2 \tau P'(\tau) \) and \( \mathcal{M}_S(\tau) = 2 \tau S'(\tau) \) with the prime denoting a derivative with respect to \( \tau \).
In the case of the diphoton partial widths, one has

$$\Delta^\gamma = \frac{\alpha_s}{\pi} \left( A_\phi(y_{\gamma\gamma}) + M_\phi(r_3^2) \ln \frac{\mu_B^2}{m_q^2} \right),$$

(A22)

with [54]

$$A_\rho(y) = -\frac{y(1+y^2)}{(1-y)^3 (1+y)} \left[ 72 Li_4(y) + 96 Li_4(-y) - \frac{128}{3} [Li_3(y) + Li_3(-y)] \ln y 
+ \frac{28}{3} Li_2(y) \ln^2 y + \frac{16}{3} Li_2(-y) \ln^2 y + \frac{1}{18} \ln^4 y + \frac{8}{3} \zeta_2 \ln^2 y + \frac{32}{3} \zeta_3 \ln y + 12 \zeta_4 \right] 
+ \frac{y}{(1-y)^2} \left[ -\frac{56}{3} Li_3(y) - \frac{64}{3} Li_3(-y) + 16 Li_2(y) \ln y + \frac{32}{3} Li_2(-y) \ln y 
+ \frac{20}{3} \ln(1-y) \ln^2 y - \frac{8}{3} \zeta_2 \ln y + \frac{8}{3} \zeta_3 \right] + \frac{2y(1+y)}{3(1-y)^3} \ln^3 y,$$

(A23)

$$A_5(y) = -\frac{y(1+y+y^2+y^3)}{(1-y)^5} \left[ 108 Li_4(y) + 144 Li_4(-y) - 64 [Li_3(y) + Li_3(-y)] \ln y 
+ 14 Li_2(y) \ln^2 y + 8 Li_2(-y) \ln^2 y + \frac{1}{12} \ln^4 y + 4 \zeta_2 \ln^2 y + 16 \zeta_3 \ln y + 18 \zeta_4 \right] 
+ \frac{y(1+y^2)}{(1-y)^4} \left[ -32 Li_3(-y) + 16 Li_2(-y) \ln y - 4 \zeta_2 \ln y \right] - \frac{4y(7-2y+7y^2)}{(1-y)^4} Li_3(y) 
+ \frac{8y(3-2y+3y^2)}{(1-y)^4} Li_2(y) \ln y + \frac{2y(5-6y+5y^2)}{(1-y)^4} \ln(1-y) \ln^2 y + \frac{y(3+25y-7y^2+3y^3)}{3(1-y)^5} \ln^3 y 
+ \frac{4y(1-14y+y^2)}{(1-y)^4} \zeta_3 + \frac{12y^2}{(1-y)^3} \ln^2 y - \frac{12y(1+y)}{(1-y)^3} \ln y - \frac{20y}{(1-y)^7}. $$

(A24)

Above the $b\bar{b}$ threshold, the assumption that the new spin-0 states decay into bottom-quark pairs only through mixing with the corresponding QCD bound states becomes inadequate. Following Ref. [45], we interpolate between the resonance region and the region where perturbative QCD is applicable using a heuristic model that is inspired by QCD sum rules. The interpolations take the form

$$N^p_b = 1 - \exp \left[ -7.39 \left( 1 - \left( \frac{m_B + m_{B'}}{m_p^2} \right)^2 \right)^{2.5} \right],$$

(A25)

$$N^s_b = 1 - \exp \left[ -8.63 \left( 1 - \left( \frac{4m_B^2}{m_S^2} \right) \right)^{0.8} \right],$$

(A26)

with $m_B = 5.28$ GeV and $m_{B'} = 5.33$ GeV [41]. These expressions update the results obtained previously in Refs. [45,46]. In practice, the interpolation is achieved by multiplying the partonic decay widths $\Gamma(P, S \to b\bar{b})$ by the factors $N_{p,s}^b$ introduced above.

The partial decay widths of the spin-0 bottomonium states to gluons are given to LO in $\alpha_s$ and $v_b$ by (see for example Refs. [43,45,46])

$$\Gamma(\eta_b(n) \to gg) = \frac{\alpha_s^2}{3m_{\eta_b(n)}^2} |R_{\eta_b(n)}(0)|^2,$$

(A27)

$$\Gamma(\chi_b(n) \to gg) = \frac{3\alpha_s^2}{m_{\chi_b(n)}^2} |R'_{\chi_b(n)}(0)|^2.$$

(A28)

The partial decay widths to gluons essentially saturate the total decay widths for $\eta_b(n)$ with $n \neq 5, 6$ and all the $\chi_b(n)$ states. In the case of $\eta_b(5)$ and $\eta_b(6)$, however, also decays to final states involving $\pi$ and $B_{(s)}$ mesons are relevant. We use [41]

$$\Gamma(\eta_b(5) \to \pi \text{ mesons}) = 1.5 \text{ MeV},$$

(A29)

$$\Gamma(\eta_b(6) \to \pi \text{ mesons}) = 3 \text{ MeV},$$

(A30)

for the decays to pion final states, while the $B_{(s)}$ decays are incorporated via the approximate relations [46]
Such an approach leads to the following unitarity bounds. To get an order of magnitude estimate of the QED contributions to the dimuon branching ratios of spin-0 bottomonium states, the above formulas are hence sufficient.

Besides QED contributions, the dimuon rates of the \( \eta_b(n) \) and \( \chi_b(n) \) mesons also receive purely EW corrections associated to virtual Z-boson and Higgs exchange. Assuming again that the branching ratios to gluon pairs fully dominate, we obtain

\[
\text{Br}(\eta_b(n) \to Z^* \to \mu^+ \mu^-) = \frac{9G_F^2}{\pi \alpha_s^2} m^2_{\eta_b(n)} m^2_{\mu} \beta_{\mu/\eta_b(n)},
\]

(A37)

\[
\text{Br}(\chi_b(n) \to h^* \to \mu^+ \mu^-) = \frac{9G_F^2}{\pi \alpha_s^2} m^2_{\chi_b(n)} m^2_{\mu} \beta_{\mu/\chi_b(n)} \frac{m^4_{\chi_b(n)}}{m^4_h}.
\]

(A38)

Here \( G_F = 1.167 \times 10^{-5} \text{ GeV}^{-2} \) denotes the Fermi constant. The latter formulas can be shown to agree with results obtained in the context of \( \pi^0 \) and \( K^0 \) decays (cf. Refs. [58,59]).