

Model-independent probes of CP violation in the heavy scalar sector at muon colliders

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We propose a model-independent test of CP violation in the scalar sector. We consider a heavy neutral scalar h_2 with tree-level couplings at the $h_2 VV$ and $h_2 h_1 Z$ vertices (with $V = W^\pm, Z$), alongside the 125 GeV SM-like Higgs boson h_1 . At future muon colliders, we exploit vector-boson fusion production of h_2 followed by the decay $h_2 \rightarrow Zh_1$. In our framework, observing the single process $VV \rightarrow h_2 \rightarrow Zh_1$ implies both relevant couplings are nonzero, which is sufficient to establish CP violation in the scalar sector. We simulate signal and backgrounds at $\sqrt{s} = 3(10)$ TeV with integrated luminosity $L = 0.9(10)$ ab^{-1} . We then present the expected discovery sensitivities across the $(c_2 \text{ and } c_{12})$ parameter space (with the coupling parameters c_2 and c_{12} defined in the text) for multiple m_{h_2} hypotheses.

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I. INTRODUCTION

CP violation was first discovered in 1964 in the rare decay of the long-lived kaon, $K_L \rightarrow \pi^+ \pi^-$ [1]. Additional CP -violating effects have since been measured in meson and baryon systems [2–7]. In the standard model (SM), CP violation arises solely from the Kobayashi-Maskawa (KM) mechanism [8], equivalently the complex phase of the Cabibbo-Kobayashi-Maskawa matrix [8,9]. The KM mechanism successfully describes all established CP -violating observables [6,10,11]. However, it cannot account for the observed matter-antimatter asymmetry of the Universe [12–14], motivating searches for new sources of CP violation beyond the SM (BSM).

In the SM there is no CP violation originating from the scalar sector. Theoretically, many BSM scenarios introduce additional sources of CP violation, especially in models with an extended scalar sector [15–19]. In such models, the Higgs boson(s) can be CP mixed and thereby exhibit CP -violating interactions. Experimentally, most of these scenarios already face strict constraints from electric dipole moment (EDM) measurements of the electron, neutron, atoms, etc. [20–23], because they typically predict EDMs much larger than in the SM [24–30]. However, EDMs alone

cannot distinguish different CP violation sources, so direct probes of CP -violating interactions at colliders are also essential.¹

The discovery of the 125 GeV SM-like Higgs boson (denoted h_1 below) at the Large Hadron Collider (LHC) [67–69] marked a turning point in particle physics, making tests of its CP properties crucial for elucidating the Higgs sector. Current data are consistent with a purely CP -even h_1 , but a CP -mixed h_1 is not excluded [47]. In models with an extended scalar sector, there can be additional states $h_{2,3,4,\dots}$ (h_i with $i > 1$), whose possible CP mixing leads to rich collider signatures.

As a representative example, CP violation in the Yukawa sector has been widely studied. For a CP -mixed scalar h_i coupled to fermions via

$$\mathcal{L} \supset -h_i \bar{f}(g_S + ig_P \gamma^5)f, \quad (1.1)$$

one typically considers $f = t$ [47–50,58,70–88] or $f = \tau$ [32,52,53,89–97], since the spin information of t or τ is imprinted in final-state distributions and is sensitive to the CP nature of h_i . Observation of both CP -even and CP -odd components of h_i would confirm CP violation. Such an idea to test CP violation is effective for both the 125 GeV Higgs boson ($i = 1$) or an additional scalar ($i > 1$).

CP violation can also be probed purely in the bosonic sector through interactions of scalars with the massive SM gauge bosons $W^\pm$ and Z , as proposed in Ref. [98].

¹These two complementary avenues have generated a rich phenomenology of CP violation in BSM scenarios, see, e.g., Refs. [31–66] for details.

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To employ this method at tree level, at least two scalars must be discovered—the effective interaction can be written as [98]

$$\mathcal{L} \supset \left(\frac{g^2 v}{2} W^{+\mu} W_{\mu}^{-} + \frac{g^2 v}{4c_W^2} Z^{\mu} Z_{\mu} \right) \left(\sum_i c_i h_i \right) + \sum_{i < j} \frac{c_{ij} g}{2c_W} Z_{\mu} (h_i \partial^{\mu} h_j - h_j \partial^{\mu} h_i), \quad (1.2)$$

where g is the weak gauge coupling, $v = 246$ GeV is the vacuum expectation value (VEV) of the SM Higgs doublet, and $c_W \equiv \cos \theta_W$ is the cosine of the Weinberg angle θ_W . The parameters c_i denote the $h_i VV$ coupling strengths relative to the SM, and for the SM-like Higgs boson h_1 , we have $c_1 \simeq 1$. For any two distinct scalars h_i and h_j , the quantity $K \equiv c_i c_j c_{ij}$ serves as a measure of CP violation [19,98,99]. Since nonzero c_i implies a CP -even component in h_i , and nonzero c_{ij} implies that h_i and h_j contain components of the opposite CP number, $K \neq 0$ is a sufficient condition to establish CP violation. Recent collider studies employing this method include Refs. [43,46,98,100].

In this paper we focus on CP violation in the pure bosonic sector following Ref. [98]. Reference [98] considers a light extra scalar h_2 and prospects at a Higgs factory with $\sqrt{s} = 250$ GeV (e.g., CEPC [101–103]), however, light new states are already tightly constrained. We, therefore, study a heavy h_2 scenario with $m_{h_2} \sim \mathcal{O}(\text{TeV})$. We consider future muon colliders (MuCs) [104–110] with $\sqrt{s}$ up to 10 TeV, where TeV-scale scalars are kinematically accessible. Specifically, we study vector-boson fusion (VBF) production with $h_2 \rightarrow Zh_1$, i.e., $VV \rightarrow h_2 \rightarrow Zh_1$ with $V = W^{\pm}, Z$. Observation of this single process implies $c_2 \neq 0$ and $c_{12} \neq 0$ simultaneously, thereby probing CP violation in the scalar sector.

The paper is organized as follows. In Sec. II we describe our model-independent method to search for CP violation. In Sec. III we present the simulation setup and analysis.

In Sec. IV we show the results. Conclusions are given in Sec. V, with additional details in Appendices A–C.

II. MODEL-INDEPENDENT METHOD

Assuming that a heavy neutral scalar h_2 has been discovered, following Ref. [98], we write the tree-level effective interaction as

$$\mathcal{L} \supset \left(\frac{g^2 v}{2} W^{+\mu} W_{\mu}^{-} + \frac{g^2 v}{4c_W^2} Z^{\mu} Z_{\mu} \right) (c_1 h_1 + c_2 h_2) + \frac{c_{12} g}{2c_W} Z_{\mu} (h_1 \partial^{\mu} h_2 - h_2 \partial^{\mu} h_1), \quad (2.1)$$

without further assumptions on the ultraviolet (UV) complete model. Since $c_1 \simeq 1$, CP violation can be confirmed if both c_2 and c_{12} are nonzero, as discussed above. It is then natural to study the VBF processes $VV \rightarrow h_2 \rightarrow Zh_1$ with $V = W^{\pm}, Z$ at MuC, whose Feynman diagrams are shown in Fig. 1.

In these processes, h_2 is produced via the $h_2 VV$ vertex, giving a total cross section $\sigma_{VV \rightarrow h_2} \propto c_2^2$, and subsequently decays through the $h_1 h_2 Z$ vertex with branching ratio $\text{Br}_{h_2 \rightarrow Zh_1} \equiv \Gamma_{h_2 \rightarrow Zh_1} / \Gamma_{h_2} \propto c_{12}^2 / \Gamma_{h_2}$, where Γ_{h_2} denotes the total decay width of h_2 . If either $c_2 = 0$ or $c_{12} = 0$, then $\sigma_{VV \rightarrow h_2} \cdot \text{Br}_{h_2 \rightarrow Zh_1} = 0$ and the process is absent, conversely, the observation of such a process implies $c_2 c_{12} \neq 0$ and hence CP violation in the scalar sector. We compute $\sigma_{VV \rightarrow h_2}$ at future MuCs with $\sqrt{s} = 3$ and 10 TeV, respectively, using MadGraph5_aMC@NLO (v3.6.2) [111], and show its dependence on m_{h_2} in Fig. 2 (left). For given m_{h_2} and $\sqrt{s}$, the cross section of W^+W^- fusion is about an order larger than that of ZZ fusion, which means that W^+W^- fusion is the dominant process. For $c_2 \simeq 0.2$, which is a typical benchmark point in the following analysis, the total cross section $\sigma_{VV \rightarrow h_2} \propto c_2^2$ can reach at most $\mathcal{O}(1 - 10)$ fb in the mass region considered in this work, and decreases quickly as m_{h_2} increases.

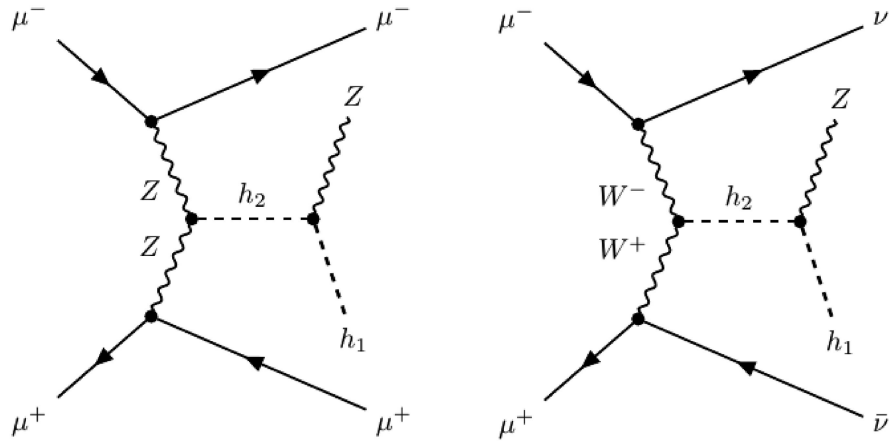


FIG. 1. Feynman diagrams for the VBF processes $VV \rightarrow h_2 \rightarrow Zh_1$ (with $V = W^{\pm}, Z$).

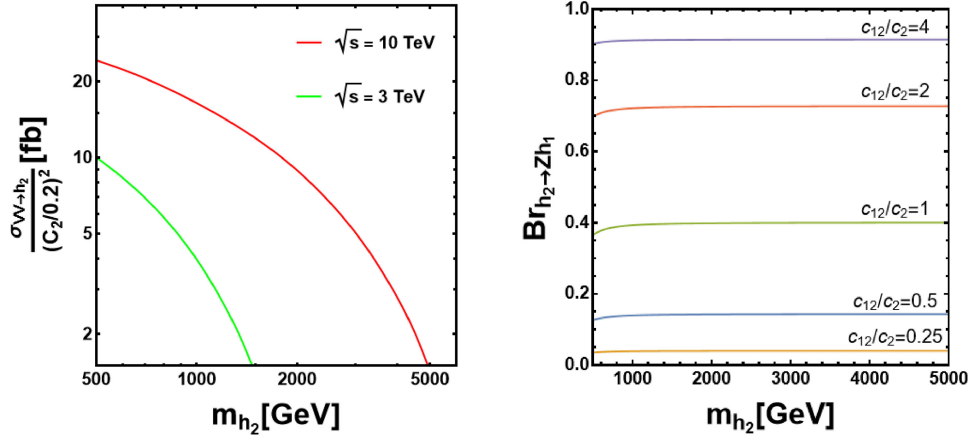


FIG. 2. Left: total cross sections σ of $VV \rightarrow h_2$ at future MuCs with $\sqrt{s} = 3$ and 10 TeV as a function of m_{h_2} . Right: $\text{Br}_{h_2 \rightarrow Zh_1}$ as a function of m_{h_2} for different c_{12}/c_2 .

We assume that Eq. (2.1) contains all the interactions related to h_2 , and thus h_2 decays only through the following three channels: $h_2 \rightarrow Zh_1$, $h_2 \rightarrow ZZ$, and $h_2 \rightarrow W^+W^-$. The branching ratio for the decay channel $h_2 \rightarrow Zh_1$ is defined as

$$\text{Br}_{h_2 \rightarrow Zh_1} \equiv \frac{\Gamma_{h_2 \rightarrow Zh_1}}{\Gamma_{h_2}} = \frac{\Gamma_{h_2 \rightarrow Zh_1}}{\Gamma_{h_2 \rightarrow Zh_1} + \Gamma_{h_2 \rightarrow W^+W^-} + \Gamma_{h_2 \rightarrow ZZ}}, \quad (2.2)$$

where the partial decay widths are given as [19,112,113]

$$\Gamma_{h_2 \rightarrow W^+W^-} = \frac{m_{h_2}^3 c_2^2}{16\pi v^2} \sqrt{1 - \frac{4m_W^2}{m_{h_2}^2}} \left(1 - \frac{4m_W^2}{m_{h_2}^2} + \frac{12m_W^4}{m_{h_2}^4} \right), \quad (2.3)$$

$$\Gamma_{h_2 \rightarrow ZZ} = \frac{m_{h_2}^3 c_2^2}{32\pi v^2} \sqrt{1 - \frac{4m_Z^2}{m_{h_2}^2}} \left(1 - \frac{4m_Z^2}{m_{h_2}^2} + \frac{12m_Z^4}{m_{h_2}^4} \right), \quad (2.4)$$

$$\Gamma_{h_2 \rightarrow Zh_1} = \frac{m_{h_2}^3 c_{12}^2}{16\pi v^2} f^3 \left(\frac{m_Z^2}{m_{h_2}^2}, \frac{m_{h_1}^2}{m_{h_2}^2} \right). \quad (2.5)$$

Here, $m_{h_1, h_2, Z, W}$ denote the corresponding particle masses, and the function

$$f(x, y) \equiv \sqrt{1 + x^2 + y^2 - 2x - 2y - 2xy}. \quad (2.6)$$

If $m_{h_2} \gg m_{h_1, W, Z}$, the total decay width of h_2 approximately behaves as

$$\Gamma_{h_2} \simeq (493c_2^2 + 329c_{12}^2) \left(\frac{m_{h_2}}{1 \text{ TeV}} \right)^3 \text{ GeV}. \quad (2.7)$$

Numerically, Fig. 2 (right) shows $\text{Br}_{h_2 \rightarrow Zh_1}$ as a function of m_{h_2} for different ratios c_{12}/c_2 . The branching ratio is sensitive to c_{12}/c_2 but only weakly dependent on m_{h_2} .

In particular, in the limit $m_{h_2} \gg m_{h_1, W, Z}$, we have approximately

$$\text{Br}_{h_2 \rightarrow Zh_1} \simeq \frac{2(c_{12}/c_2)^2}{2(c_{12}/c_2)^2 + 3}, \quad (2.8)$$

which is nearly independent on m_{h_2} .

III. SIMULATION STUDIES

A. Simulation setup

In this work, we study the VBF processes $VV \rightarrow h_2 \rightarrow Z(\rightarrow \ell^+ \ell^-) h_1(\rightarrow b \bar{b})$ with $V = W^\pm, Z$ and $\ell = e, \mu$ at the MuC, assuming that a heavy h_2 has already been discovered. The effective interaction in Eq. (2.1) is implemented with FeynRules (v2.0) [114] to produce a Universal FeynRules Output (UFO) model, which we load in MadGraph5_aMC@NLO (v3.6.2) [111] to simulate the $\mu^- \mu^+$ collisions, and generate events for the whole processes of both signal and backgrounds. Event generation is then interfaced to PYTHIA8.3 [115] for parton showering and hadronization. Detector response is simulated with Delphes 3.4.2 [116] using a muon collider configuration card.

An absorber is installed at the MuC to mitigate beam-induced backgrounds (BIBs), so only objects within $10^\circ < \theta < 170^\circ$ are reconstructed, where θ denotes the polar angle with respect to the z -axis (the initial μ^- beam direction) [117–120]. Objects produced in the very forward/backward regions are absorbed and thus considered to be undetected in this study.

We must treat jets in this work, because the signal we consider here includes two b -jets, and we must also consider the background processes including b -jets or light jets, which are mis-tagged as b -jets. For jet reconstruction, we use the algorithm of “VLCjetR05N2” [121–124]. The double- b -tagging efficiency is approximately 0.8, while the probability to mis-tag non- b -jets as two b -jets can reach about $\mathcal{O}(10^{-2})$ [124].

B. Signal and background processes

At future MuCs, we target the VBF processes $VV \rightarrow h_2 \rightarrow h_1 Z$ to search for CP violation in the scalar sector, as shown in Fig. 1. For most events from the ZZ fusion topology (left panel of Fig. 1), the scattered muons emerge at very small polar angles and low transverse momentum p_T and, therefore, are outside the detector acceptance. We select $Z \rightarrow \ell^- \ell^+$ (with $\ell = e, \mu$) and $h_1 \rightarrow b\bar{b}$. For $W^+ W^-$ fusion, the final state contains two energetic neutrinos, which are undetectable, while for ZZ fusion, the final state contains two energetic $\mu^\pm$, which appear in the very forward/backward region in most events, and thus cannot be detected as well. Hence, we generate the two VBF topologies together, in which the final state contains large missing energy, two opposite-charge, same-flavor leptons, and two b -tagged jets.

The signal generation cross section σ_{sig} scales with a parameter

$$\kappa \equiv c_2^2 \cdot \text{Br}_{h_2 \rightarrow Zh_1}, \quad (3.1)$$

and thus depends on m_{h_2} , c_2 , and c_{12} . In the limit $m_{h_2} \gg m_{h_1, W, Z}$, we have approximately $\kappa \simeq \frac{2c_2^2 c_{12}^2}{3c_2^2 + 2c_{12}^2}$ based on the results in Eqs. (2.3)–(2.5). For the chosen final state, the cross section is also proportional to the SM branching

fractions [6]

$$\text{Br}_{Z \rightarrow \ell^- \ell^+} = 0.033647 \quad \text{and} \quad \text{Br}_{h_1 \rightarrow b\bar{b}} = 0.5824. \quad (3.2)$$

Global fits to the 125 GeV Higgs signal strength data show that $c_1 \gtrsim 0.95$ at 95% C.L. [47] assuming no exotic h_1 decay channels.² Even under the assumption of custodial symmetry in the Higgs sector [6], the sum rule on the couplings c_1 , c_2 , and c_{12} still depends on the UV-complete model construction, especially the weak hypercharge of the extended scalar sector. In Appendix A, we derive it in a simplified scenario. Following the sum rule, we typically choose the parameter region as $c_2^2 + c_{12}^2 \lesssim 1 - c_1^2 \lesssim 0.1$, which is still allowed by current LHC data, and thus for the phenomenological studies, we choose the parameter regions $c_2 \leq 0.2$ and $c_{12} \leq 0.2$ as benchmarks.³ Direct LHC searches for a heavy scalar decaying to ZZ final state further constrain c_2 for $m_{h_2} \lesssim 700$ GeV [125], and thus we choose all the benchmark points with $m_{h_2} \gtrsim 700$ GeV due to the consistency with LHC bounds.⁴

We consider two center-of-mass energies of the $\mu^- \mu^+$ collisions, $\sqrt{s} = 3$ and 10 TeV. The corresponding integrated luminosities are $L = 0.9$ and 10 ab^{-1} , respectively [104]. To generate the signal samples, we choose the following benchmark points:

$$m_{h_2} \in \begin{cases} \{700, 1000\} \text{ GeV}, & (\text{for } \sqrt{s} = 3 \text{ TeV}), \\ \{700, 1000, 1500, 2000, 3000, 4500\} \text{ GeV}, & (\text{for } \sqrt{s} = 10 \text{ TeV}). \end{cases} \quad (3.3)$$

All signal events are generated with the parameter choice $c_2 = c_{12} = 0.2$, which leads to the largest allowed width of h_2 , to ensure that our search strategy works in the whole parameter region with $(c_2, c_{12}) \leq 0.2$.

Given the final state containing undetected forward/backward muons or neutrinos, two opposite-charge, same-flavor leptons, and two b -tagged jets (including the mis-tagged non- b -jets), we consider four main backgrounds:

- (i) $VV \rightarrow h_2 \rightarrow Z(\rightarrow \ell^- \ell^+) Z(\rightarrow jj)$, which is a typical BSM background process, labeled “b1” with cross section σ_{b1} . Here, σ_{b1} scales with a parameter

$$\xi \equiv c_2^2 \cdot \text{Br}_{h_2 \rightarrow ZZ}, \quad (3.4)$$

where

$$\begin{aligned} \text{Br}_{h_2 \rightarrow ZZ} &\equiv \frac{\Gamma_{h_2 \rightarrow ZZ}}{\Gamma_{h_2}} \\ &= \frac{\Gamma_{h_2 \rightarrow ZZ}}{\Gamma_{h_2 \rightarrow Zh_1} + \Gamma_{h_2 \rightarrow W^+ W^-} + \Gamma_{h_2 \rightarrow ZZ}}. \end{aligned} \quad (3.5)$$

In the limit $m_{h_2} \gg m_{h_1, W, Z}$, we have approximately

$\xi \simeq \frac{c_2^4}{3c_2^2 + 2c_{12}^2}$ based on the results in Eqs. (2.3)–(2.5).

- (ii) $\mu^- \mu^+ \rightarrow \nu \bar{\nu} Z(\rightarrow \ell^- \ell^+) h_1(\rightarrow b\bar{b})$ and $\mu^- \mu^+ \rightarrow \ell^- \ell^+ Z(\rightarrow \ell^- \ell^+) h_1(\rightarrow b\bar{b})$, labeled “b2” with cross section σ_{b2} .
- (iii) $\mu^- \mu^+ \rightarrow \nu \bar{\nu} Z(\rightarrow \ell^- \ell^+) Z(\rightarrow jj)$ and $\mu^- \mu^+ \rightarrow \ell^- \ell^+ Z(\rightarrow \ell^- \ell^+) Z(\rightarrow jj)$, labeled “b3” with cross section σ_{b3} .
- (iv) $\mu^- \mu^+ \rightarrow b\bar{b} W^-(\rightarrow \bar{\nu} \ell^-) W^+(\rightarrow \nu \ell^+)$, labeled “b4” with cross section σ_{b4} .

²The global fits in [47] were performed based on the two-Higgs-doublet model (2HDM), but the data strongly favor the SM-like limit, and hence the constraint on c_1 depends weakly on the specific UV-complete model assumptions. On the other hand, $c_1 \simeq 0.95$ is still allowed by LHC data.

³In this paper, we only discuss the case $c_2, c_{12} > 0$ for simplicity.

⁴Note that the direct LEP bounds on (c_2, c_{12}) quoted in Ref. [98] were derived for a light scalar (e.g., $m_2 = 40$ GeV), which is kinematically accessible at LEP (and assuming scalar decays dominantly to $b\bar{b}$), and hence do not apply to our TeV-scale h_2 benchmarks.

The total cross section of backgrounds is defined as $\sigma_{\text{bkg}} \equiv \sigma_{\text{b1}} + \sigma_{\text{b2}} + \sigma_{\text{b3}} + \sigma_{\text{b4}}$.

Background events are generated with the same tools and settings as the signal. To maintain consistency, event yields are estimated from the MadGraph5_aMC@NLO (v3.6.2) [111] production cross sections. Note that b1 is a BSM background process, whose cross section depends on the parameters m_{h_2} , c_2 , and c_{12} , while b2–b4 are all SM background processes, whose cross sections do not depend on the BSM parameters.

C. Analysis strategy

1. Preselection

Final-state leptons and b -jets are ordered by descending transverse momentum and labeled O_i ($i = 1, 2, \dots$), with $O \in \{\ell, b\text{-jet}\}$. We apply the following preselection cuts to select the target final state and reject background at the first stage:

- (i) Exactly two opposite-charge, same-flavor leptons, i.e., $N(\ell) = 2$ with $\ell = e, \mu$.
- (ii) Exactly two b -tagged jets, i.e., $N(j_b) = 2$.

Jets do not carry a well-defined electric charge—the so-called “jet charge” is an estimator and is not used here to require “opposite charges” for b -jets [126–128]. The second condition will miss the events in which two b -jets are not fully tagged, and include the events in which light jets are mis-tagged as two b -jets, as discussed above.

2. Reconstruction

In the signal topology, the heavy h_2 decays to one SM Higgs h_1 and one Z boson, subsequently $Z \rightarrow \ell^+ \ell^-$ and $h_1 \rightarrow b\bar{b}$. We reconstruct the h_2 mass from the invariant mass of the $\ell^+ \ell^- b\bar{b}$ system, $m_{b\bar{b}\ell^-\ell^+}$, and the h_1 mass from the invariant mass of the two b -jets, $m_{b\bar{b}}$. The two undetected energetic forward/backward objects (neutrinos or absorbed muons) form the invisible system, and we define its invariant mass as $\cancel{m}$, which captures the VBF kinematic features in both signal and some background processes. In our detailed study, we find that setting selection cuts on $m_{b\bar{b}}$ and $m_{b\bar{b}\ell^-\ell^+}$ is enough to separate signal and background events, and thus $\cancel{m}$ is only used as a tagging condition for VBF processes.

In this section, we choose two benchmark points: (i) $m_{h_2} = 700$ GeV with $\sqrt{s} = 3$ TeV and (ii) $m_{h_2} = 3000$ GeV with $\sqrt{s} = 10$ TeV, to show how the selection cuts are set for the observables, $m_{b\bar{b}}$ and $m_{b\bar{b}\ell^-\ell^+}$, together with the total cross sections for both signal and background after the selection cuts. Details for the other six benchmark points are found in the Appendices.

In Fig. 3, we choose the benchmark point (i), and show the normalized distributions of $m_{b\bar{b}}$, $m_{b\bar{b}\ell^-\ell^+}$, and $\cancel{m}$, for both signal and background processes after preselection. Based on the left plot, we choose the selection cut

$100 \text{ GeV} \leq m_{b\bar{b}} \leq 140 \text{ GeV}$, which is effective to suppress backgrounds b1, b3, and b4. In background b2, the $b\bar{b}$ pairs also come from h_1 , meaning that its distribution should be similar to that of the signal process. Based on the middle plot, we choose the selection cut $640 \text{ GeV} \leq m_{b\bar{b}\ell^-\ell^+} \leq 720 \text{ GeV}$,⁵ which is effective to suppress backgrounds b2, b3, and b4. Since b1 is a BSM background, which also comes from the h_2 decay, the $m_{b\bar{b}\ell^-\ell^+}$ distribution in b1 should be similar to that of the signal process. If we perform these two selection cuts together, it is efficient to suppress all four background processes. We also show the distribution of $\cancel{m}$ distributions as a VBF tagging condition, however, it cannot provide further separation between the signal and background processes after we set selection cuts on $m_{b\bar{b}}$ and $m_{b\bar{b}\ell^-\ell^+}$. After selection cuts, we have the total cross sections for both signal and background processes as

$$\sigma_{\text{sig}} = 1.58\kappa \text{ (fb)} \quad \text{and} \quad \sigma_{\text{bkg}} = (14\xi + 5.1) \times 10^{-3} \text{ (fb)}, \quad (3.6)$$

which can be used to predict the discovery potential of this process for given model parameters (c_2 , c_{12}) and integrated luminosity L , with $m_{h_2} = 700$ GeV.

In Fig. 4, we choose the benchmark point (ii), and show the normalized distributions of $m_{b\bar{b}}$, $m_{b\bar{b}\ell^-\ell^+}$, and $\cancel{m}$, for both signal and background processes after preselection. Based on the left plot, the distributions of $m_{b\bar{b}}$ for both signal and background processes are quite similar to those in the case of benchmark point (i), so we choose the selection cut $100 \text{ GeV} \leq m_{b\bar{b}} \leq 140 \text{ GeV}$ again. Based on the middle plot, it can be found that the signal peak is much wider than that for benchmark point (i), and we choose the selection cut $2400 \text{ GeV} \leq m_{b\bar{b}\ell^-\ell^+} \leq 3400 \text{ GeV}$. Cuts on $\cancel{m}$ in the right plot cannot provide further separation between signal and background processes after selection cuts on $m_{b\bar{b}}$ and $m_{b\bar{b}\ell^-\ell^+}$, whose behavior is similar to that in benchmark point (i). After selection cuts, we have the total cross sections for both signal and background processes as

$$\sigma_{\text{sig}} = 1.13\kappa \text{ (fb)} \quad \text{and} \quad \sigma_{\text{bkg}} = (17\xi + 7.07) \times 10^{-3} \text{ (fb)}. \quad (3.7)$$

More details are shown in the Appendices. For the other six benchmark points, we show the normalized distributions

⁵The minimal necessary width of the cut window, which relates closely to the dispersion in $m_{b\bar{b}\ell^-\ell^+}$ distribution, is sensitive to both the energy smearing at detector level and the total width of h_2 (especially for large m_{h_2}), denoted as Γ_{h_2} , which is calculated in Eq. (2.7). In this work, all signal events are generated using the benchmark point $c_2 = c_{12} = 0.2$, leading to the largest allowed Γ_{h_2} , which ensures our search strategy works in the whole parameter region we consider.

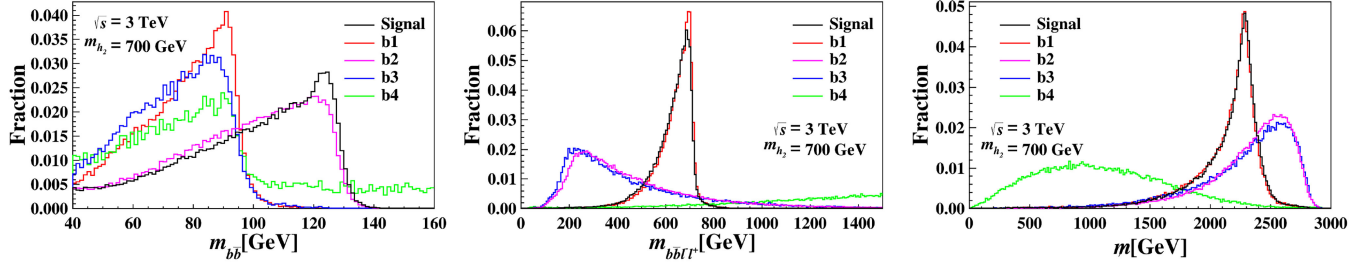


FIG. 3. Normalized distributions of $m_{b\bar{b}}$ (left), $m_{b\bar{b}l\ell^+}$ (middle), and m (right), for both signal and background processes after preselection ($m_{h_2} = 700$ GeV with $\sqrt{s} = 3$ TeV).

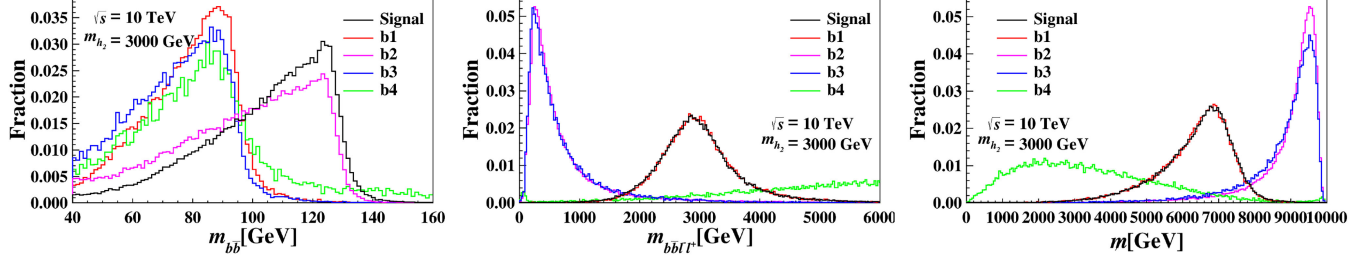


FIG. 4. Normalized distributions of $m_{b\bar{b}}$ (left), $m_{b\bar{b}l\ell^+}$ (middle), and m (right), for both signal and background processes after preselection ($m_{h_2} = 3000$ GeV with $\sqrt{s} = 10$ TeV).

of $m_{b\bar{b}}$, $m_{b\bar{b}l\ell^+}$, and m in Appendix B. Following these distributions, we set the selection cuts on $m_{b\bar{b}}$ and $m_{b\bar{b}l\ell^+}$ for all the eight benchmark points. The selection cuts on $m_{b\bar{b}}$ are the same for all the eight benchmark points, $100 \text{ GeV} \leq m_{b\bar{b}} \leq 140 \text{ GeV}$, while the selection cuts on $m_{b\bar{b}l\ell^+}$ are sensitive to m_{h_2} , as shown in Table I. For all the eight benchmark points, m cannot be used to separate signal and background processes further after setting selection cuts on $m_{b\bar{b}}$ and $m_{b\bar{b}l\ell^+}$, thus it is only used as VBF tagging.

Following the analysis procedure above, we show the cross sections for both signal and background processes for all the eight benchmark points, after each step (initial production, preselection cuts, and selection cuts), in Appendix C. For background processes, we show both σ_{b1-b4} separately and the total cross section σ_{bkg} . If $(c_2, c_{12}) \leq 0.2$, we have $\xi \simeq \frac{c_2^4}{3c_2^2 + 2c_{12}^2} \lesssim 1.3 \times 10^{-2}$, and thus for each benchmark point, the dominant background after selection cuts should be b2.

IV. RESULTS

The expected event numbers of signal and background processes after selection cuts are

$$N_{\text{sig}} = \sigma_{\text{sig}} L \quad \text{and} \quad N_{\text{bkg}} = \sigma_{\text{bkg}} L, \quad (4.1)$$

where L is the integrated luminosity. The statistical significance is quantified through

$$\sigma_{\text{stat}} = \sqrt{2 \left[(N_{\text{sig}} + N_{\text{bkg}}) \ln \left(1 + \frac{N_{\text{sig}}}{N_{\text{bkg}}} \right) - N_{\text{sig}} \right]}, \quad (4.2)$$

which increases as $L^{1/2}$. Based on the analysis above, we present the expected discovery potential for CP violation in the scalar sector at muon colliders with $\sqrt{s} = 3(10)$ TeV and the corresponding integrated luminosity $L = 0.9(10) \text{ ab}^{-1}$, in Figs. 5 and 6.

TABLE I. Selection cuts on $m_{b\bar{b}l\ell^+}$ for all the eight benchmark points.

m_{h_2} (GeV)	700	1000	700	1000
$\sqrt{s}$ (TeV)	3	3	10	10
$m_{b\bar{b}l\ell^+}$ Cut (GeV)	640–720	920–1020	640–720	920–1020
m_{h_2} (GeV)	1500	2000	3000	4500
$\sqrt{s}$ (TeV)	10	10	10	10
$m_{b\bar{b}l\ell^+}$ Cut (GeV)	1300–1600	1700–2200	2400–3400	3400–5400

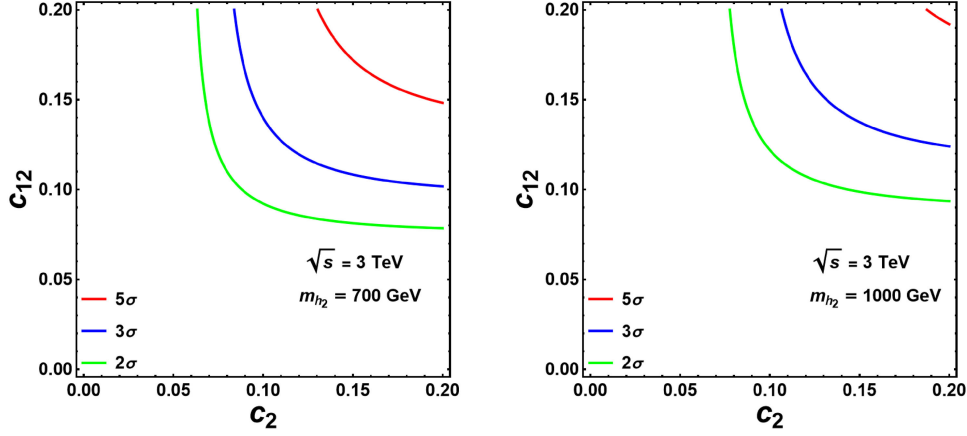


FIG. 5. Expected discovery potential for significance for points in the (c_2, c_{12}) plane with $\sqrt{s} = 3$ TeV and $L = 0.9$ ab^{-1} . Benchmark points: $m_{h_2} \in \{700, 1000\}$ GeV. The colored lines correspond to the boundaries with expected 2σ (green), 3σ (blue), and 5σ (red) significances, respectively.

For a MuC with $\sqrt{s} = 3$ TeV and corresponding integrated luminosity $L = 0.9$ ab^{-1} , assuming both $(c_2, c_{12}) \lesssim 0.2$, CP violation in the scalar sector can be discovered at the 5σ level up to $m_{h_2} \simeq 1$ TeV. For larger m_{h_2} , the cross section decreases quickly, which leads to the weaker discovery potential. While for a MuC with $\sqrt{s} = 10$ TeV and corresponding integrated luminosity $L = 10$ ab^{-1} , assuming both $(c_2, c_{12}) \lesssim 0.2$, CP violation in the scalar sector can be discovered at the 5σ level up to $m_{h_2} \simeq 4.5$ TeV, because of the larger cross section and integrated luminosity. When $m_{h_2} \lesssim 3$ TeV, the discovery potential changes slowly, and the case with parameters $(c_2, c_{12}) \simeq 0.1$ can be discovered at the 5σ level. The results show significant advantages for future MuCs to test CP violation in the scalar sector, especially for the heavy h_2 scenario.

V. CONCLUSIONS AND DISCUSSIONS

We propose a model-independent strategy to test CP violation in an extended scalar sector at future MuCs. The key observation is the existence of the single process

$$VV \rightarrow h_2 \rightarrow Zh_1 \quad (\text{with } V = W^\pm, Z). \quad (5.1)$$

It already requires both couplings $c_2 \neq 0$ and $c_{12} \neq 0$. Therefore, an observation of this channel is sufficient to establish CP violation in the scalar sector within the effective framework of Eq. (2.1). The absorbers installed to mitigate BIBs [117–120] imply that the signal receives contributions from both W^+W^- and ZZ fusion, because the very forward/backward $\mu^\pm$ cannot be detected and thus behave as missing energy.

In our collider study, we focus on the clean final state $Z(\rightarrow \ell^+\ell^-)h_1(\rightarrow b\bar{b})$, exploit the reconstructed masses $m_{b\bar{b}\ell^-\ell^+}$ and $m_{b\bar{b}}$, and use simple, robust selections to suppress backgrounds. After selection cuts, the dominant

background is $b\bar{b}$ for all benchmark points, while $b1$ is efficiently suppressed by the $m_{b\bar{b}}$ cut and the smallness of ξ and $\text{Br}_{Z \rightarrow b\bar{b}}$. The sensitivity trends obtained at $\sqrt{s} = 3$ and 10 TeV (with the respective integrated luminosities $L = 0.9$ and 10 ab^{-1} used in Sec. III) show that the VBF topology offers competitive discovery reach for a wide range of $m_{h_2} \sim \mathcal{O}(\text{TeV})$ at future MuCs. Especially for the $\sqrt{s} = 10$ TeV future MuC with $L = 10$ ab^{-1} , $(c_2, c_{12}) \simeq 0.1(0.2)$ can be discovered at the 5σ level up to a rather heavy $m_{h_2} \lesssim 3(4.5)$ TeV.

Our analysis targets the multi-TeV regime where VBF processes naturally benefit from the logarithmic enhancement of gauge boson radiation, making the MuC an efficient “gauge boson collider.” The considered MuC parameters $\sqrt{s}$ and L are consistent with current community road maps and interim reports for a staged MuC program [108,110]. Within this context, the $VV \rightarrow h_2 \rightarrow Zh_1$ channel provides a direct handle on CP violation that is complementary to EDM constraints and to Yukawa-sector probes discussed in Sec. I. Importantly, our selection is compatible with realistic machine-detector interface conditions at the MuC, where forward/backward shielding against BIB [117–120] motivates restricted angular acceptance in the final states.

In this work, we focus on a general h_2 interaction in Eq. (2.1), without assuming a UV-complete model, targeting this special type of CP violation in the heavy scalar sector. The main limitation of this method is that we must first discover the additional scalar h_2 , and it must interact with the Z -boson and SM-like Higgs boson h_1 at tree level, following Eq. (2.1). Once these conditions are satisfied, this method is universal for BSM models that contain one or more heavy scalar(s) with such type of interactions. As mentioned in Ref. [98], some CP -conserving neutral states h_2 may also interact with VV and Zh_1 at loop level. However, such scenarios are distinguishable from the case we discuss in this paper, because loop-induced effective

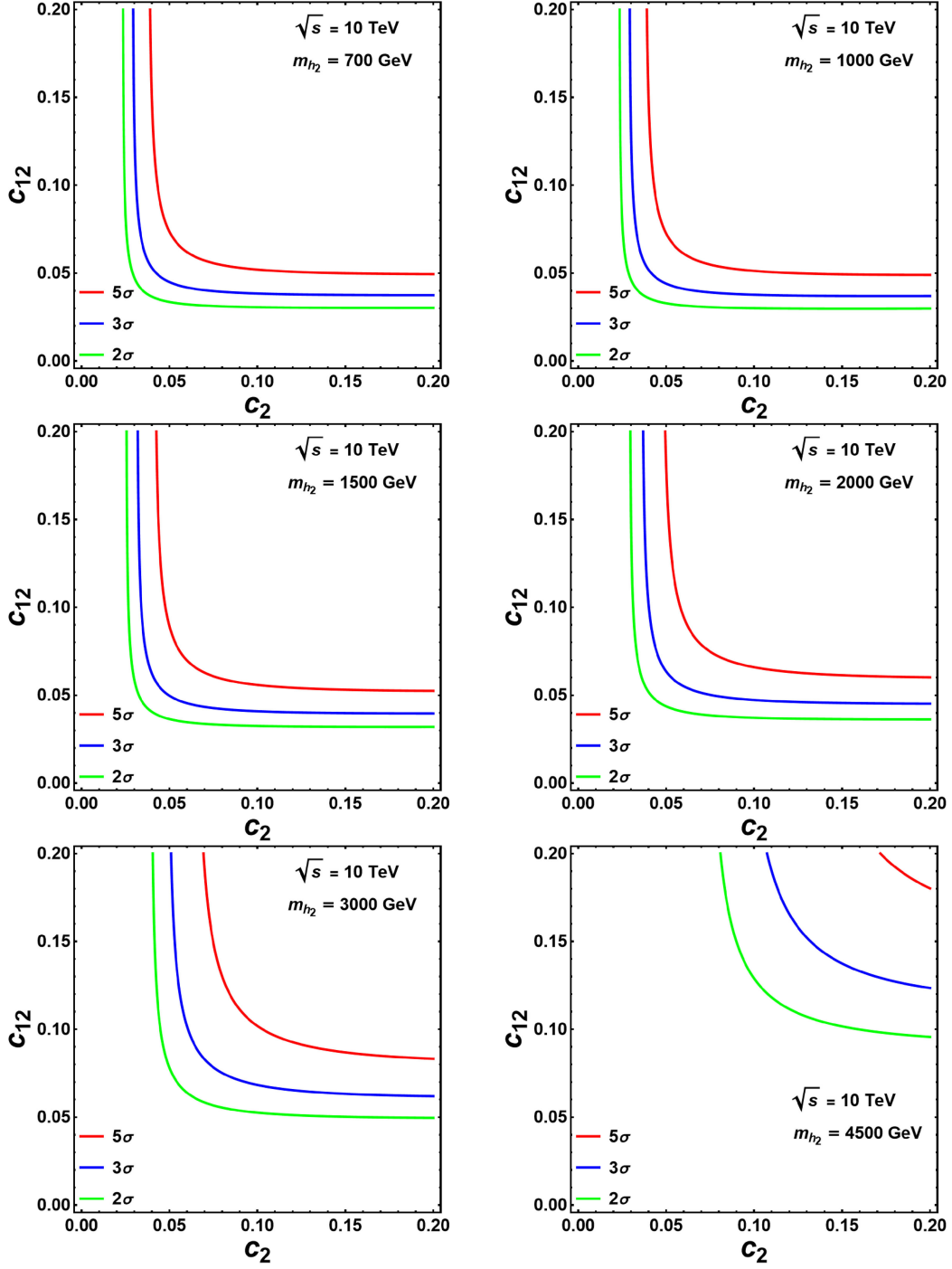


FIG. 6. Expected discovery potential for significance for points in the (c_2, c_{12}) plane with $\sqrt{s} = 10$ TeV and $L = 10 \text{ ab}^{-1}$. Benchmark points: $m_{h_2} \in \{700, 1000, 1500, 2000, 3000, 4500\}$ GeV. The colored lines correspond to the boundaries with expected 2σ (green), 3σ (blue), and 5σ (red) significances, respectively.

interactions always lead to small enough cross sections, corresponding to an effective $(c_2, c_{12}) \lesssim \mathcal{O}(10^{-2})$. That means our method at the MuC is sufficient to confirm CP violation in the scalar sector.

In this work, we did not consider h_2 interactions beyond Eq. (2.1). In a specific UV-complete model, h_2 of course may interact with other SM particles (depending strongly on the concrete model construction), which may lead to rich phenomenology. For example, as discussed in Sec. I, if h_2 interact with fermions, it may also lead to CP violation effects in the Yukawa sector. Since we focus on the specific type of CP violation in this paper in a model-independent way without further assumptions on the UV-complete model, here we do not discuss other CP violation effects beyond the interaction (2.1), and we leave such studies to some forthcoming projects. If h_2 has the interactions beyond Eq. (2.1), there will also be additional decay channels of h_2 , which will modify the total width of h_2 in Eq. (2.7) and hence the decay branching ratio $\text{Br}_{h_2 \rightarrow Zh_1}$. It will not break the effectiveness of the method, but modifies the detailed discovery potential shown in Sec. IV a bit.

In summary, observing $VV \rightarrow h_2 \rightarrow Zh_1$ with the selections outlined in this work would constitute compelling evidence for CP violation in the scalar sector. Conversely, the nonobservation can be translated into robust, model-independent bounds on the coupling combination (c_2, c_{12}) , providing a clear target for future MuC programs.

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Note added. Following standard practice in high-energy physics, authors are listed in strict alphabetical order by surname. This ordering should not be interpreted as indicating any ranking of contribution, seniority, or leadership. All authors contributed equally to this work.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not

technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: SUM RULE FOR THE COUPLINGS c_1 , c_2 , AND c_{12} IN A SIMPLIFIED SCENARIO

Generally, for a scalar multiplet ϕ_I with the weak isospin I and weak hypercharge Y , the electroweak covariant derivative can be written as

$$D_\mu \phi_I \equiv \left(\partial_\mu - ig W_\mu^a \tau_I^a - ig' \frac{Y}{2} B_\mu \right) \phi_I, \quad (\text{A1})$$

where g, g' are gauge coupling constants, and W_μ^a and B_μ are gauge fields of $\text{SU}(2)_L$ and $\text{U}(1)_Y$ groups separately. ϕ_I forms a $2I + 1$ -plet of the $\text{SU}(2)_L$ group, which must be a complex field if $Y \neq 0$. τ_I^a are three generators of the $\text{SU}(2)_L$ group in the representation of dimension $2I + 1$ —for $I = 1/2$, τ_I^a become the Pauli matrices. We usually choose τ_I^3 diagonal as

$$\tau_I^3 = \text{diag}\{I, I - 1, \dots, 1 - I, -I\}. \quad (\text{A2})$$

For a component of ϕ_I , we denote it as ϕ_{I_3} , which contains the isospin third component I_3 . The covariant derivative containing the neutral gauge fields can be written as

$$\begin{aligned} D_\mu \phi_{I_3} &\supset \left[\partial_\mu - ig I_3 (s_W A_\mu + c_W Z_\mu) \right. \\ &\quad \left. - ig' \frac{Y}{2} (c_W A_\mu - s_W Z_\mu) \right] \phi_{I_3} \\ &= \left[\partial_\mu - i|e| \left(I_3 + \frac{Y}{2} \right) A_\mu \right. \\ &\quad \left. - i \frac{g}{c_W} \left(I_3 c_W^2 - \frac{Y}{2} s_W^2 \right) Z_\mu \right] \phi_{I_3}. \end{aligned} \quad (\text{A3})$$

Here, $s_W(c_W) \equiv \sin \theta_W(\cos \theta_W)$, and A_μ is the photon field. Based on Eq. (A3), we straightforwardly have the extension of the Gell-Mann-Nishijima relation to the electroweak interaction as $Q = I_3 + Y/2$. For a neutral component ϕ_{I_3} , we have $I_3 = -Y/2$, and thus the covariant derivative (A3) is reduced to

$$D_\mu \phi_{I_3} \supset \left(\partial_\mu + i \frac{gY}{2c_W} Z_\mu \right) \phi_{I_3}, \quad (\text{A4})$$

depending on the weak hypercharge Y .

Assuming custodial symmetry in the Higgs sector, we restrict to the simplified case where the scalar VEVs appear only in $\text{SU}(2)_L$ singlets or doublets [6]. Here, we set the VEVs of all other types of Higgs multiplets as zero for simplicity. For all the neutral singlets, since $I = Y = 0$,

they cannot lead to interactions with SM gauge bosons like in Eq. (2.1). In any UV-complete model, no matter how many scalar doublets it contains, we can always perform a rotation among the doublets, to ensure only one of the doublets contains a VEV, and we then denote it as ϕ_{SM} , which contains the dominant component of h_1 . In a general model, the extended scalar sector may be very complex. However, we can consider a simplified scenario, in which only one extended scalar multiplet ϕ_I contributes to the interaction (2.1) significantly, or equivalently, h_2 mainly comes from ϕ_I . In this scenario, the neutral scalar sector contains

$$\phi_{\text{SM}} \supset \frac{v_{\text{SM}} + h}{\sqrt{2}} \quad \text{and} \quad \phi_I \supset \phi_{I_3} = \frac{H + iH'}{\sqrt{2}}. \quad (\text{A5})$$

In the basis (A5), the h component contributes only to hVV coupling, while the H and H' components contribute only to the $HH'Z$ coupling, as

$$\begin{aligned} \mathcal{L} \supset & \left(\frac{g^2 v}{2} W^{+\mu} W_{\mu}^{-} + \frac{g^2 v}{4c_W^2} Z^{\mu} Z_{\mu} \right) h \\ & + \frac{gY}{2c_W} Z_{\mu} (H \partial^{\mu} H' - H' \partial^{\mu} H). \end{aligned} \quad (\text{A6})$$

The scalar mass eigenstates $h_{1,2,3}$ can be defined through an orthogonal matrix $\mathcal{R}$ (whose elements are defined as $\mathcal{R}_{ij}$) as

$$(h_1, h_2, h_3) = (h, H, H') \mathcal{R}^T. \quad (\text{A7})$$

Comparing with Eq. (2.1), we straightforwardly have

$$\begin{aligned} c_1 &= \mathcal{R}_{11}, \quad c_2 = \mathcal{R}_{21}, \\ c_{12} &= Y(\mathcal{R}_{12}\mathcal{R}_{23} - \mathcal{R}_{13}\mathcal{R}_{22}) = Y\mathcal{R}_{31}. \end{aligned} \quad (\text{A8})$$

$Y = 0$ leads to a vanishing c_{12} , equivalently, $c_{12} \neq 0$ requires $|Y|$ to be a positive integer. We then obtain the sum rule of the couplings as

$$c_1^2 + c_2^2 + \frac{c_{12}^2}{Y^2} = 1. \quad (\text{A9})$$

It means that the sum rule for the couplings c_1 , c_2 , and c_{12} is sensitive to the UV-complete model. As an example, for the 2HDM, which requires $|Y| = 1$, we simply have $c_1^2 + c_2^2 + c_{12}^2 = 1$. For any $|Y| \geq 1$, the parameter region $c_2^2 + c_{12}^2 < 1 - c_1^2$ is still not excluded by experiments, and thus we can typically choose such benchmarks in the text.

APPENDIX B: ADDITIONAL RECONSTRUCTION DISTRIBUTIONS

We show the normalised distributions of the observables $m_{b\bar{b}}$, $m_{b\bar{b}\ell^-\ell^+}$, and $\hat{m}$ in Fig. 7 for the other six benchmark points as mentioned above.

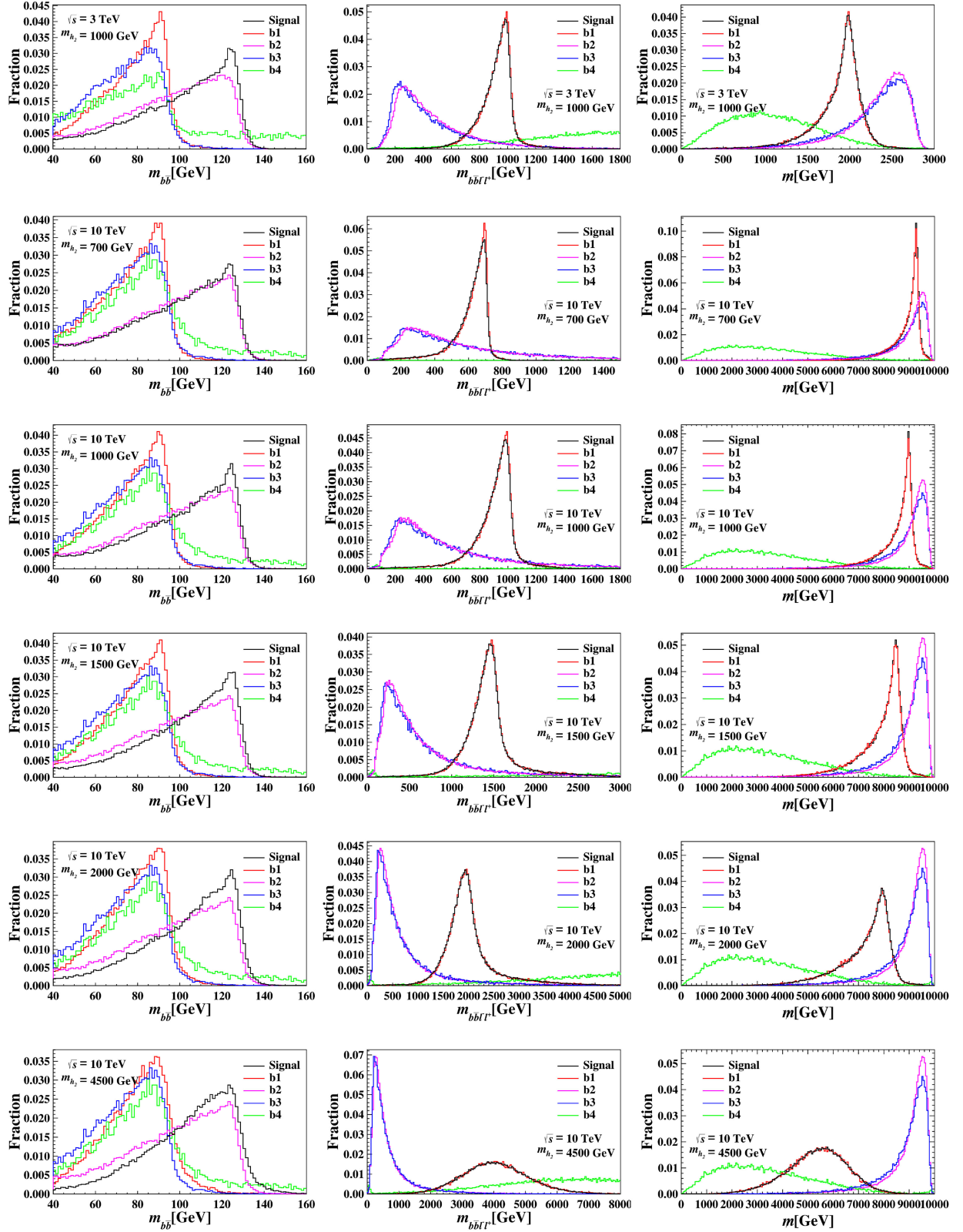


FIG. 7. Normalized distributions of the observables $m_{b\bar{b}}$ (left), $m_{b\bar{b}\ell\ell^*}$ (middle), and m (right), for all the other six benchmark points from top to bottom: $m_{h_2} = 1000$ GeV with $\sqrt{s} = 3$ TeV, and $m_{h_2} = 700, 1000, 1500, 2000, 4500$ GeV with $\sqrt{s} = 10$ TeV.

APPENDIX C: CROSS SECTIONS AFTER EACH STEP

We show the cross sections for both signal and background processes after each step: initial production (denoted as “ini.”), preselection cuts (denoted as “pre-sel.”), and selection cuts (denoted as “sel.”). Results for the two benchmark points with $\sqrt{s} = 3$ TeV are shown in Table II, and results for the six benchmark points with $\sqrt{s} = 10$ TeV are shown in Table III.

TABLE II. Cross sections for signal and background processes after each step (initial production, preselection cuts, and selection cuts) for benchmark points with $\sqrt{s} = 3$ TeV.

m_{h_2} (GeV)	cuts	σ_{sig} (fb)	σ_{bkg} (fb)	σ_{b1} (fb)	σ_{b2} (fb)	σ_{b3} (fb)	σ_{b4} (fb)
700	ini.	6.75κ	$8.16\xi + 5.5$	8.16ξ	0.39	2.71	2.40
	pre-sel.	4.13κ	$1.12\xi + 0.96$	1.12ξ	0.18	0.34	0.44
	sel.	1.58κ	$0.014\xi + 0.0051$	0.014ξ	0.0045	0.00035	0.00025
1000	ini.	3.90κ	$4.68\kappa + 5.5$	4.68κ	0.39	2.71	2.40
	pre-sel.	2.49κ	$0.72\xi + 0.96$	0.72ξ	0.18	0.34	0.44
	sel.	0.86κ	$0.007\xi + 0.0028$	0.007ξ	0.0022	0.00016	0.00044

TABLE III. Cross sections for signal and background processes after each step (initial production, preselection cuts, and selection cuts) for benchmark points with $\sqrt{s} = 10$ TeV. “...” means this background process is negligible with $L = 10 \text{ ab}^{-1}$.

m_{h_2} (GeV)	cuts	σ_{sig} (fb)	σ_{bkg} (fb)	σ_{b1} (fb)	σ_{b2} (fb)	σ_{b3} (fb)	σ_{b4} (fb)
700	ini.	20.12κ	$24.18\xi + 11.4$	24.18ξ	1.39	9.6	0.41
	pre-sel.	10.58κ	$3.24\xi + 1.37$	3.24ξ	0.44	0.90	0.03
	sel.	3.74κ	$0.035\xi + 0.00987$	0.035ξ	0.0092	0.00067	...
1000	ini.	16.15κ	$19.42\xi + 11.4$	19.42ξ	1.39	9.60	0.41
	pre-sel.	9.30κ	$2.83\xi + 1.37$	2.83ξ	0.44	0.90	0.03
	sel.	3.02κ	$0.038\xi + 0.00625$	0.038ξ	0.0061	0.00015	...
1500	ini.	11.76κ	$14.13\xi + 11.4$	14.13ξ	1.39	9.6	0.41
	pre-sel.	7.27κ	$2.19\xi + 1.37$	2.19ξ	0.44	0.90	0.03
	sel.	2.96κ	$0.032\xi + 0.00850$	0.032ξ	0.0084	0.00010	...
2000	ini.	8.70κ	$10.46\xi + 11.4$	10.46ξ	1.39	9.6	0.41
	pre-sel.	5.40κ	$1.62\xi + 1.37$	1.62ξ	0.44	0.90	0.03
	sel.	2.11κ	$0.025\xi + 0.00752$	0.025ξ	0.0074	0.00012	...
3000	ini.	4.93κ	$5.93\xi + 11.4$	5.93ξ	1.39	9.6	0.41
	pre-sel.	2.80κ	$0.85\xi + 1.37$	0.85ξ	0.44	0.90	0.03
	sel.	1.13κ	$0.017\xi + 0.00707$	0.017ξ	0.0069	0.00017	...
4500	ini.	1.98κ	$2.38\xi + 11.4$	2.38ξ	1.39	9.6	0.41
	pre-sel.	0.67κ	$0.21\xi + 1.37$	0.21ξ	0.44	0.90	0.03
	sel.	0.28κ	$0.007\xi + 0.00493$	0.007ξ	0.0038	0.00083	0.00030

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