

**Exclusive  $B \rightarrow PV$  decays and  $CP$  violation in the general two-Higgs-doublet model**

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We calculate all the branching ratios and direct  $CP$  violations of  $B \rightarrow PV$  decays in the most general two-Higgs-doublet model with spontaneous  $CP$  violation (type III 2HDM). As the model has rich  $CP$ -violating sources, it is shown that the new physics effects to direct  $CP$  violations and branching ratios in some channels can be significant when adopting the generalized factorization approach to evaluate the hadronic matrix elements, which provides good signals for probing new physics beyond the SM in the future  $B$  experiments.

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**I. INTRODUCTION**

To reveal the origin of  $CP$  violation is an important subject not only for exploring the basic symmetry of space-time and new physics beyond the standard model (SM), but also for understanding the matter-antimatter asymmetry in the evolution of universe. It is well known that  $CP$  violation in the SM is characterized by a single weak phase in the Cabibbo-Kobayashi-Maskawa (CKM) matrix [1], which can provide a satisfied explanation for the direct  $CP$  violation  $\varepsilon'/\varepsilon$  [2] established in kaon decays [3], and also direct  $CP$  violation [4] observed in  $B$ -meson decays [5]. Though the theory of the strong and electro-weak (EW) interactions in SM has met with extraordinary success, it is widely believed that the SM can not be the final theory of particle physics, in particular, because the Higgs sector of SM is not well understood yet and the  $CP$  phase in CKM matrix is not enough to understand the baryon and antibaryon asymmetry in the universe. Many possible extensions of SM in Higgs sector have been proposed [6] and it was suggested that  $CP$  symmetry may break down spontaneously [7]. Other possible extensions of the SM have been explored, such as the super symmetric model (SUSY) [8], little Higgs model [9] and extra dimensions [10], which all make better the situation of the SM. But at present, no single model is good enough to solve all the problems existing in the SM and it is then worthwhile to consider all the possibilities beyond SM. One of the simplest extensions of the SM, the so-called two-Higgs-doublet model (2HDM) which introduces an extra Higgs doublet without imposing the *ad hoc* discrete symmetries has been investigated widely from various considerations [11–20]. Motivated solely from the origin of  $CP$  violation (CPV), a general two-Higgs-doublet model with spontaneous  $CP$  violation (type III 2HDM) has been shown to provide one of the simplest and attractive models in understanding the origin and mechanism of  $CP$  violation at weak scale [15,16]. In such a model, there exists more

physical neutral and charged Higgs bosons and rich  $CP$ -violating sources from a single  $CP$  phase of vacuum. In particular, the type III 2HDM which allows flavor-changing neutral currents (FCNCs) at tree level but suppressed by approximate  $U(1)$  flavor symmetry has attracted more interests and is very different from the so-called type I and type II 2HDM in which an *ad hoc* discrete symmetry ( $Z_2$  symmetry) has been imposed to avoid the FCNCs. In fact, the type I and type II 2HDM can be regarded as special cases of the type III 2HDM.

It is known that the FCNCs concerning the first two generations are highly suppressed from low-energy experiments, and those involving the third generation is not as severely suppressed as the first two generations. Thus the type III 2HDM can be parameterized in a way to satisfy the current experimental constraints. The constraints on type III 2HDM from neutral meson mixings ( $K^0 - \bar{K}^0$ ,  $D^0 - \bar{D}^0$ ,  $B^0 - \bar{B}^0$ ) [21] and radiative decays of bottom quark [22–24] have been studied in details. In this paper, we investigate the new physics influences of the type III 2HDM on two-body charmless nonleptonic  $B$  decays  $B \rightarrow PV$  with  $P, V$  denoting the pseudoscalar and vector mesons, respectively. Because these decays have triggered considerable theoretical interest in understanding SM and they are also thought to be sensitive and important in exploring new physics beyond the SM as they involve the so-called tree (current-current)  $b \rightarrow (u, c)$  and/or  $B \rightarrow (d, s)$  penguin amplitudes with both QCD and electroweak penguin transition participating. In the two-Higgs-doublet model, there are four additional physical Higgs bosons except the  $H^0$  Higgs in SM. As the couplings involving Higgs bosons and fermions have complex  $CP$  phases in type III 2HDM,  $CP$ -violating effects occur even in the simplest case that all the tree-level FCNC couplings are negligible. With the improvement of experimental precision, more and more direct  $CP$  violation have been observed and will be much precisely tested in the future experiments.

This paper is organized as follows. In Sec II, we describe the theoretical frame including a brief introduction of the two-Higgs-doublet model with spontaneous  $CP$  violation,

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i.e., type III 2HDM, and the effective Hamiltonian as well as the generalized factorization formula, which is our basic tool to estimate the branching ratios and  $CP$  violation of  $B$  meson decays. In Sec III, we make a detailed calculation of  $B \rightarrow PV$  decays with  $P$  denoting the pseudoscalar meson and  $V$  the vector meson using the generalized factorization formula and give out quantitative predictions. Our conclusions and discussions are presented in the last section.

## II. THEORETICAL FRAMEWORK

### A. Outline of two-Higgs-doublet model

One of the important developments of SM is the so-called Higgs mechanism, i.e., a spontaneous symmetry breaking mechanism by which the gauge bosons and fermions can get their masses. In SM, a single Higgs doublet of  $SU(2)$  is introduced to break the  $SU(2)_L \times U(1)_Y$  symmetry to  $U(1)_{em}$  and generate masses to the gauge bosons and fermions. Nevertheless, the physics Higgs boson predicted by SM has not been experimentally tested although enormous efforts have been made and SM gives no explanation of the origin of  $CP$  violation. The theoretical defects of SM itself suggests the existence of new physics. Many attempts have been made by both theorists and experimen-

talists to explore the mechanisms of  $CP$  violation since the discovery of  $CP$  violation in 1964. It was suggested that  $CP$  symmetry can be broken spontaneously, which requires at least two Higgs doublets [7]. A consistent and simple model which provides a spontaneous  $CP$  violation mechanism was constructed completely in a general Two-Higgs-doublet model [15,16] without the *ad hoc* discrete symmetry, which is called model III. Such a model not only explains the origin of  $CP$  violation in the SM, but also induces rich new resources of  $CP$  violation. These new sources of  $CP$  violation can lead to some significant phenomenological effects which are promising to be tested by the future  $B$  factory and LHCb. In this note, we will focus on the phenomenological applications of the type III 2HDM in the two-body charmless hadronic  $B \rightarrow PV$  decays.

The two complex Higgs doublets in the type III 2HDM are expressed as [15–17,19,20]:

$$\phi_1 = \begin{pmatrix} \phi_1^\dagger \\ \phi_1^0 \end{pmatrix}, \quad \phi_2 = \begin{pmatrix} \phi_2^\dagger \\ \phi_2^0 \end{pmatrix}. \quad (1)$$

The corresponding Higgs potential can simply be written as the following general form:

$$\begin{aligned} V(\phi) = & \lambda_1(\phi_1^\dagger \phi_1 - \frac{1}{2}v_1^2)^2 + \lambda_2(\phi_2^\dagger \phi_2 - \frac{1}{2}v_2^2)^2 + \lambda_3(\phi_1^\dagger \phi_1 - \frac{1}{2}v_1^2)(\phi_2^\dagger \phi_2 - \frac{1}{2}v_2^2) + \lambda_4[(\phi_1^\dagger \phi_2)(\phi_2^\dagger \phi_1)] \\ & + \frac{1}{2}\lambda_5(\phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_1 - v_1 v_2 \cos \delta)^2 + \lambda_6(\phi_1^\dagger \phi_2 - \phi_2^\dagger \phi_1 - v_1 v_2 \sin \delta)^2 \\ & + [\lambda_7(\phi_1^\dagger \phi_1 - \frac{1}{2}v_1^2)^2 + \lambda_8(\phi_2^\dagger \phi_2 - \frac{1}{2}v_2^2)^2][\phi_1^\dagger \phi_2 + \phi_2^\dagger \phi_1 - v_1 v_2 \cos \delta], \end{aligned} \quad (2)$$

where  $\lambda_i (i = 1, 2, \dots, 8)$  are all real parameters. If all  $\lambda_i$  are non-negative, the minimum occurs at

$$\langle \phi_1^0 \rangle = v_1 e^{i\delta}, \quad \langle \phi_2^0 \rangle = v_2. \quad (3)$$

With  $v_1, v_2$  are the vacuum expectation values of  $\phi_1, \phi_2$  respectively, and  $\delta$  the relative phase of the vacuum. It is clear that in the above potential,  $CP$  nonconservation can only occur through the vacuum with  $\delta \neq 0$ . Obviously, such a  $CP$  violation appears as an explicit one in the potential when  $\lambda_6 \neq 0$  [16].

After a unitary transformation, it is natural and convenient to use the following basis:

$$H_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} \sqrt{2}G^+ \\ v + \phi_1^0 + iG^0 \end{bmatrix}, \quad H_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} \sqrt{2}H^+ \\ \phi_2^0 + iA^0 \end{bmatrix}, \quad (4)$$

with

$$\langle H_1^0 \rangle = v e^{i\delta}, \quad \langle H_2^0 \rangle = 0, \quad (5)$$

where  $v = \sqrt{v_1^2 + v_2^2}$  and is related to the  $W$  mass by  $M_W = gv/2$ . Here  $H^0$  plays the role of the Higgs boson in the standard model.  $H^\pm$  are the charged scalar pair with  $H^\pm = \sin\beta \phi_1^\pm e^{-i\delta} - \cos\beta \phi_2^\pm$ , where  $\tan\beta = v_2/v_1$ . As for the neutral Higgs,  $\phi_1, \phi_2$  are not the mass eigenstates

but can be expressed as linear combinations of  $CP$ -even neutral Higgs mass eigenstates  $H_0$  and  $h_0$  through

$$\begin{aligned} H_0 &= \phi_1^0 \cos\alpha + \phi_2^0 \sin\alpha, \\ h_0 &= -\phi_1^0 \sin\alpha + \phi_2^0 \cos\alpha, \end{aligned} \quad (6)$$

where  $\alpha$  is the mixing angle and when  $\alpha = 0$ ,  $(\phi_1^0, \phi_2^0)$  are identical with  $(H_0, h_0)$ . For simplicity, the mixing with the pseudoscalar  $A^0$  is not considered here.

Let us consider a Yukawa Lagrangian of the following form:

$$\begin{aligned} \mathcal{L}_Y = & \xi_{1ij}^U \bar{Q}_{i,L} \tilde{\phi}_1 U_{j,R} + \xi_{1ij}^D \bar{Q}_{i,L} \phi_1 D_{j,R} \\ & + \xi_{2ij}^U \bar{Q}_{i,L} \tilde{\phi}_2 U_{j,R} + \xi_{2ij}^D \bar{Q}_{i,L} \phi_2 D_{j,R} + \text{H.c.}, \end{aligned} \quad (7)$$

where  $\phi_i (i = 1, 2)$  are the two Higgs doublets,  $\tilde{\phi}_{1,2} = i\tau_2 \phi_{1,2}^*$ ,  $Q_{i,L} (U_{j,R})$  with  $i = (1, 2, 3)$  are the left-handed isodoublet quarks (right-handed up-type quarks),  $D_{j,R}$  are the right-handed isosinglet down-type quarks, while  $\xi_{1ij}^{U,D}$  and  $\xi_{2ij}^{U,D}$  ( $i, j = 1, 2, 3$  are family index) are generally the nondiagonal matrices of the Yukawa coupling. After diagonalizing the mass matrix of quark fields, the Yukawa Lagrangian related to the decays we considered in this paper can be written as

$$\begin{aligned}
\mathcal{L}_Y = & -\frac{g}{2M_W}(H^0 \cos\alpha - h^0 \sin\alpha)(\bar{U}M_U U + \bar{D}M_D D) \\
& -\frac{H^0 \sin\alpha + h^0 \cos\alpha}{\sqrt{2}} \left[ \bar{U} \left( \xi^U \frac{1}{2}(1 + \gamma_5) + \xi^{U\dagger} \frac{1}{2}(1 - \gamma_5) \right) U + \bar{D} \left( \xi^D \frac{1}{2}(1 + \gamma_5) + \xi^{D\dagger} \frac{1}{2}(1 - \gamma_5) \right) D \right] \\
& + \frac{iA^0}{\sqrt{2}} \left[ \bar{U} \left( \xi^U \frac{1}{2}(1 + \gamma_5) - \xi^{U\dagger} \frac{1}{2}(1 - \gamma_5) \right) U - \bar{D} \left( \xi^D \frac{1}{2}(1 + \gamma_5) - \xi^{D\dagger} \frac{1}{2}(1 - \gamma_5) \right) D \right] \\
& - H^+ \bar{U} \left[ V_{\text{CKM}} \xi^D \frac{1}{2}(1 + \gamma_5) - \xi^{D\dagger} \frac{1}{2}(1 - \gamma_5) \right] D - H^- \bar{D} \left[ \xi^{D\dagger} V_{\text{CKM}}^\dagger \frac{1}{2}(1 - \gamma_5) - V_{\text{CKM}}^\dagger \xi^U \frac{1}{2}(1 + \gamma_5) \right] U, \quad (8)
\end{aligned}$$

where  $U$  represents the mass eigenstates of up-type quarks  $U = (u, c, t)$  quarks and  $D$  represents the mass eigenstates of down-type quarks  $D = (d, s, b)$  quarks,  $V_{\text{CKM}}$  is the Cabibbo-Kobayashi-Maskawa matrix and  $\hat{\xi}^{U,D}$  are the FCNC couplings in the mass eigenstate, and they may be parameterized as follows in terms of the quark mass:

$$\begin{aligned}
\xi_{ij}^{U,D} &= \lambda_{ij} \frac{g\sqrt{m_i m_j}}{\sqrt{2}M_W}, \quad \hat{\xi}^U = \xi^U \cdot V_{\text{CKM}}, \\
\hat{\xi}^D &= V_{\text{CKM}} \cdot \xi^D. \quad (9)
\end{aligned}$$

From the above parameterization scheme, we can see that tree-level FCNCs relating to the first two generations are naturally suppressed by the small quark masses, but are not severely suppressed in the third generation transitions. In this paper, we choose  $\xi^{U,D}$  to be diagonal, i.e.  $\xi_{ii}^{U,D} \equiv \xi_i^{U,D}$  ( $i = s, c, b, t$ ), and neglect the first generation quarks' contributions. Thus the leading contribution arises from the diagram with a top quark in the loop and the relevant couplings will be  $\hat{\xi}_{ts}^{U,D}$  and  $\hat{\xi}_{tb}^{U,D}$ , their explicit form is

$$\begin{aligned}
\hat{\xi}_{ts}^U &= \xi_t^U V_{ts}, & \hat{\xi}_{tb}^U &= \xi_t^U V_{tb} \\
\hat{\xi}_{ts}^D &= \xi_s^D V_{ts}, & \hat{\xi}_{tb}^D &= \xi_b^D V_{tb}. \quad (10)
\end{aligned}$$

Then  $\lambda_{ij}(i, j = s, c, t, b)$  and the masses of five Higgs bosons are the basic free parameters in the general two-Higgs-doublet model. Their numerical values should be constrained through experiments. It is interesting to investigate the possible constraints on the parameter space for the type III 2HDM as the FCNCs can appear at tree level. The main constraints on these parameters are from the direct measurements of the observables such as:  $R_b$ ,  $\rho$  and the electric dipole moments(EDM) at LEP experiments, and from the measurements of the neutral meson mixings  $F^0 - \bar{F}^0$  with  $F^0 = K^0, B_d^0$ . One of the most stringent constraints arises from the radiative decay of  $B$  mesons and also from the inclusive decay of bottom quark  $b \rightarrow s\gamma$  which has the least hadronic uncertainties. Since the aim of this paper is to estimate the new physics effect on the process  $B \rightarrow PV$ , we shall consider the input parameters of the type III 2HDM in a rather large range allowed by the current experiments.

In the type III 2HDM with spontaneous  $CP$  violation, the induced  $CP$  violation can be classified into the following four types via their interactions [15,16]: (i) from the

CKM matrix; (ii) from the charged Higgs couplings to the fermions  $\xi_{\text{charged}}$ ; (iii) from the neutral Higgs couplings to the fermions  $\xi_{\text{neutral}}$ ; (iv) from the  $CP$  nonconservation Higgs potential  $V(\phi)$  via mixings among scalars and pseudoscalar bosons.

## B. Effective Hamiltonian and Wilson coefficients

The effective Hamiltonian for the charmless  $B$  decays with  $\Delta B = 1$  can be expressed as

$$\begin{aligned}
\mathcal{H} = & \frac{G_F}{\sqrt{2}} \sum_{p=u,c} V_{pb} V_{ps}^* \left( C_1 Q_1^p + C_2 Q_2^p \right. \\
& + \sum_{i=3,\dots,16} [C_i Q_i + C_i' Q_i'] + C_{7\gamma} Q_{7\gamma} + C_{8g} Q_{8g} \\
& \left. + C_{7\gamma}' Q_{7\gamma}' + C_{8g}' Q_{8g}' \right) + \text{H.c.} \quad (11)
\end{aligned}$$

The definitions for the operators  $Q_{1,\dots,10}, Q_{7\gamma}, Q_{8g}$  can be found in Ref. [25]. Here the operators  $Q_1$  and  $Q_2$  are the current-current operators and  $Q_{3-6}$  are QCD penguin operators.  $Q_{7\gamma}$  and  $Q_{8g}$  are, respectively, the magnetic penguin operators for  $b \rightarrow s\gamma$  and  $b \rightarrow sg$ . Note that the mass of the external strange quark has been neglected in comparison with the external bottom-quark mass.

The additional new operators relating to the neutral Higgs mediated processes ( $b \rightarrow s\bar{q}q$  for example) are given as follows [26]:

$$\begin{aligned}
Q_{11} &= (\bar{s}b)_{(S+P)} \sum (\bar{q}q)_{(S-P)}, \\
Q_{12} &= (\bar{s}_i b_j)_{(S+P)} \sum (\bar{q}_j q_i)_{(S-P)}, \\
Q_{13} &= (\bar{s}b)_{(S+P)} \sum (\bar{q}q)_{(S+P)}, \\
Q_{14} &= (\bar{s}_i b_j)_{(S+P)} \sum (\bar{q}_j q_i)_{(S+P)}, \quad (12) \\
Q_{15} &= (\bar{s}\sigma^{\mu\nu}(1 + \gamma_5)b) \sum (\bar{q}\sigma^{\mu\nu}(1 + \gamma_5)q), \\
Q_{16} &= (\bar{s}_i\sigma^{\mu\nu}(1 + \gamma_5)b_j) \sum (\bar{q}_j\sigma^{\mu\nu}(1 + \gamma_5)q_i),
\end{aligned}$$

where  $(\bar{q}_1 q_2)_{S\pm P} = \bar{q}_1(1 \pm \gamma_5)q_2$  with  $q = u, d, s, c, b$ . The operators  $Q_i'$  in Eq. (11) are obtained from  $Q_i$  via

exchanging  $L \leftrightarrow R$ . As the primed operators's contributions are suppressed by a factor  $m_s/m_b$ , we shall neglect their effects in our present considerations. The Wilson coefficients  $C_i$ ,  $i = 1, \dots, 10$  have been calculated at the leading order (LO) [27,28] and next-to-leading order (NLO) [25] in the SM and also at the LO in the 2HDM [29,30]. For completeness, we shall list the NLO initial coefficient functions  $C_i(M_W)$  in the 2HDM [30,31]:

$$\begin{aligned}
C_1(M_W) &= \frac{11}{2} \frac{\alpha_s(M_W)}{4\pi}, \\
C_2(M_W) &= 1 - \frac{11}{6} \frac{\alpha_s(M_W)}{4\pi} - \frac{35}{18} \frac{\alpha}{4\pi}, \\
C_3(M_W) &= -\frac{\alpha_s(M_W)}{24\pi} \{\tilde{E}_0(x_t) + E_0^{III}(y)\} \\
&\quad + \frac{\alpha}{6\pi} [2B_0(x_t) + C_0(x_t)], \\
C_4(M_W) &= \frac{\alpha_s(M_W)}{8\pi} \{\tilde{E}_0(x_t) + E_0^{III}(y)\}, \\
C_5(M_W) &= -\frac{\alpha_s(M_W)}{24\pi} \{\tilde{E}_0(x_t) + E_0^{III}(y)\}, \\
C_6(M_W) &= \frac{\alpha_s(M_W)}{8\pi} \{\tilde{E}_0(x_t) + E_0^{III}(y)\}, \\
C_7(M_W) &= \frac{\alpha(M_W)}{6\pi} [4C_0(x_t) + \tilde{D}_0(x_t)], \\
C_8(M_W) &= 0, \\
C_9(M_W) &= \frac{\alpha}{6\pi} \left[ 4C_0(x_t) + \tilde{D}_0(x_t) \right. \\
&\quad \left. + \frac{1}{\sin^2\theta_W} (10B_0(x_t) - 4C_0(x_t)) \right], \\
C_{10}(M_W) &= 0,
\end{aligned} \tag{13}$$

and the LO initial Wilson coefficient functions  $C_{7\gamma}$ ,  $C_{8g}$ :

$$\begin{aligned}
C_{7\gamma}(M_W) &= -\frac{A(x_t)}{2} - \frac{A(y)}{6} |\lambda_{tt}|^2 + B(y) |\lambda_{tt}\lambda_{bb}| e^{i\theta}, \\
C_{8g}(M_W) &= -\frac{D(x_t)}{2} - \frac{D(y)}{6} |\lambda_{tt}|^2 + E(y) |\lambda_{tt}\lambda_{bb}| e^{i\theta},
\end{aligned} \tag{14}$$

where  $x_t = m_t^2/M_W^2$  and  $y = m_t^2/M_{H^{\pm 2}}$ . The explicit expressions of the Inami-Lim functions  $A, B, D, E, \dots$  in the SM and 2HDM can be found in Ref. [29].

For the new operators  $Q_{(11,12\dots 16)}$ , the corresponding initial Wilson coefficient functions  $C_i$ ,  $i = 11, \dots, 16$  at the leading order have been calculated in Refs. [26,32] and given by

$$\begin{aligned}
C_{11}(M_W) &= \frac{\alpha}{4\pi} \frac{m_b}{m_\tau \lambda_{\tau\tau}^*} (C_{Q_1} - C_{Q_2}), \\
C_{13}(M_W) &= \frac{\alpha}{4\pi} \frac{m_b}{m_\tau \lambda_{\tau\tau}} (C_{Q_1} + C_{Q_2}), \\
C_{12}(M_W) &= C_{14}(M_W) = C_{15}(M_W) = C_{16}(M_W) = 0,
\end{aligned} \tag{15}$$

The explicit expressions for  $C_{Q_1}$ ,  $C_{Q_2}$  can be found in Ref. [32].

For the  $B \rightarrow PV$  processes, the Wilson coefficient functions must run from the scale  $M_W$  to the scale of order  $O(m_b)$ . For the Wilson coefficient functions  $C_1-C_{10}$ , we shall use the results with including NLO corrections in our numerical calculations. While for  $C_{8g}$  and  $C_{7\gamma}$ , the LO results are sufficient in our present considerations. The details for the running Wilson coefficients can be found in Ref. [25]. As for the operators induced by the neutral Higgs boson, the one loop anomalous dimension matrices can be divided into two sets [26]:

$$\gamma^{RL} = \begin{array}{c|cc} & O_{11} & O_{12} \\ \hline O_{11} & -16 & 0 \\ O_{12} & -6 & 2 \end{array} \tag{16}$$

and

$$\gamma^{RR} = \begin{array}{c|cccc} & O_{13} & O_{14} & O_{15} & O_{16} \\ \hline O_{13} & -16 & 0 & 1/3 & -1 \\ O_{14} & -6 & 2 & -1/2 & -7/6 \\ O_{15} & 16 & -48 & 16/3 & 0 \\ O_{16} & -24 & -56 & 6 & -38/3 \end{array} \tag{17}$$

As the NLO Wilson coefficient functions  $C_i$ ,  $i = 11, 12, \dots, 16$  are not available now, we shall use the LO results in our numerical calculations.

### C. Generalized factorization formula

As our purpose in this paper is to evaluate the new physics effects in the type III 2HDM, it is sufficient to use the generalized factorization method [33–36] to estimate the hadronic matrix elements. It is known that in the full theory, the leading order QCD corrections to the weak transition is of the form  $\alpha_s \ln(M_W^2/p^2)$  for massless quarks, where  $p$  is the off-shell momentum of external quark lines and depends on the system under consideration. We can choose a renormalization scale  $\mu$  and separate  $\ln(M_W^2/p^2) = \ln(M_W^2/\mu^2) + \ln(\mu^2/p^2)$ . The first part  $\ln(M_W^2/\mu^2)$  is included in the Wilson coefficient functions  $c(\mu)$  which have in general summed over all leading logarithmic contributions in  $\alpha_s$  by using the renormalization group approach. While the second part involves the hadronic matrix element evaluations. It is related to the tree matrix element via

$$\langle O(\mu) \rangle = g(\mu) \langle O \rangle_{\text{tree}} \tag{18}$$

with

$$g(\mu) \sim 1 + \alpha_s(\mu) \left( \gamma \ln \frac{\mu^2}{-p^2} + c \right), \tag{19}$$

where the  $\mu$  dependence of the matrix elements is approximately extracted out to the function  $g(\mu)$ , that is

$$\langle \mathcal{H}_{\text{eff}} \rangle = c(\mu)g(\mu)\langle O \rangle_{\text{tree}} = c^{\text{eff}}\langle O \rangle_{\text{tree}}. \quad (20)$$

In principle, the effective Wilson coefficients  $c^{\text{eff}}$  should be renormalization scale independent. Thus it is necessary to incorporate QCD and EW corrections to the operators:

$$\langle O_i(\mu) \rangle = \left[ I + \frac{\alpha_s(\mu)}{4\pi} \hat{m}_s(\mu) + \frac{\alpha}{4\pi} \hat{m}_e(\mu) \right]_{ij} \langle O \rangle_{\text{tree}}, \quad (21)$$

with

$$c_i^{\text{eff}} = \left[ I + \frac{\alpha_s(\mu)}{4\pi} \hat{m}_s(\mu) + \frac{\alpha}{4\pi} \hat{m}_e^T(\mu) \right]_{ij} c_j(\mu), \quad (22)$$

The perturbative QCD and EW corrections to the matrices  $\hat{m}_s$  and  $\hat{m}_e$  from the vertex and penguin diagrams can be found in Ref. [36–38].

Using the following parameterization for the decay constants and form factors:

$$\langle 0 | A_\mu | P(q) \rangle = i f_P q_\mu, \quad \langle 0 | V_\mu | V(p, \epsilon) \rangle = f_V m_V \epsilon_\mu, \quad (23)$$

we arrive at

$$\begin{aligned} X^{BP,V} &\equiv \langle V | (\bar{q}_2 q_3)_{V-A} | \rangle \langle P | (\bar{q}_1 b)_{V-A} | B \rangle \\ &= 2 f_V m_V F_1^{B \rightarrow P}(m_V^2) (\epsilon \cdot p_B), \\ X^{BV,P} &\equiv \langle P | (\bar{q}_2 q_3)_{V-A} | \rangle \langle V | (\bar{q}_1 b)_{V-A} | B \rangle \\ &= 2 f_P m_V A_0^{B \rightarrow V}(m_P^2) (\epsilon \cdot p_B), \end{aligned} \quad (24)$$

Using the following Fierz transformation,

$$\begin{aligned} (V-A)(V+A) &\rightarrow -2(S-P)(S+P), \\ (V-A)(V-A) &\rightarrow (V-A)(V-A) \end{aligned} \quad (25)$$

one can easily obtain the tree-level matrix elements [33,35] for all the operators  $Q_{1,\dots,10}$ .

For the new operators  $Q_{11,\dots,16}$ , the additional factorization formulas must be introduced [39]:

$$\begin{aligned} \langle V(k, \epsilon^*) | \bar{q} \sigma^{\mu\nu} q' | 0 \rangle &= -i(\epsilon_\mu^* k_\nu - \epsilon_\nu^* k_\mu) f_V^\perp, \\ \langle P(p) | \bar{q} \sigma^{\mu\nu} k^\nu q' | B(p_B) \rangle &= \frac{i}{m_B + m_P} \{ q^2 (p + p_B)_\mu \\ &\quad - (m_B^2 - m_P^2) q_\mu \} f_T^P, \end{aligned} \quad (26)$$

with  $k = p_B - P$  and  $q = p_B - p$ . Where  $f_V^\perp$  and  $f_T^P$  are the tensor decay constant of vector meson and the tensor form factor relating to the  $B \rightarrow P$  transition.  $\epsilon^*$  is the polarization vector of vector meson. The hadronic matrix element is given by

$$\begin{aligned} \langle V(k, \epsilon^*) | \bar{q}' \sigma^{\mu\nu} q | 0 \rangle \langle P(p) | \bar{q} \sigma_{\mu\nu} b | B(p_B) \rangle \\ = \frac{2 f_V^\perp f_T^P m_V^2}{m_B + m_P} (\epsilon^* \cdot p_B). \end{aligned} \quad (27)$$

The tree-level matrix elements of  $Q_{(11,12,\dots,16)}$  can be factorized as ( $b \rightarrow s$ , for example):

$$\begin{aligned} \langle PV | Q_{11} | B \rangle &= a_{11} \frac{m_P^2}{(m_b + m_s)(m_q + m_{q'})} \langle P | (\bar{q}' q)_{V-A} | 0 \rangle \langle V | (\bar{s} b)_{V-A} | B \rangle, \\ \langle PV | Q_{12} | B \rangle &= -\frac{1}{2} a_{12} \langle P | (\bar{q}' q)_{V-A} | 0 \rangle \langle V | (\bar{s} b)_{V-A} | B \rangle \\ &= \frac{1}{2} a_{12} \langle V | (\bar{q}' q)_{V-A} | 0 \rangle \langle P | (\bar{s} b)_{V-A} | B \rangle, \\ \langle PV | Q_{13} | B \rangle &= -a_{13} \frac{m_P^2}{(m_b + m_s)(m_q + m_{q'})} \langle P | (\bar{q}' q)_{V-A} | 0 \rangle \langle V | (\bar{s} b)_{V-A} | B \rangle, \\ \langle PV | Q_{14} | B \rangle &= -\frac{1}{2} a_{14} \frac{m_P^2}{(m_b + m_s)(m_q + m_{q'})} \langle P | (\bar{q}' q)_{V-A} | 0 \rangle \langle V | (\bar{s} b)_{V-A} | B \rangle \\ &= \frac{1}{4} \langle V | \bar{q}' \sigma^{\mu\nu} q | 0 \rangle \langle P | \bar{s} \sigma_{\mu\nu} b | B \rangle, \\ \langle PV | Q_{15} | B \rangle &= 2 a_{15} \langle V | \bar{q}' \sigma^{\mu\nu} q | 0 \rangle \langle P | \bar{s} \sigma_{\mu\nu} b | B \rangle, \\ \langle PV | Q_{16} | B \rangle &= -a_{16} \langle V | \bar{q}' \sigma^{\mu\nu} s | 0 \rangle \langle P | \bar{q} \sigma_{\mu\nu} b | B \rangle \\ &= 6 a_{16} \frac{m_P^2}{(m_b + m_q)(m_{q'} + m_s)} \langle P | (\bar{q}' s)_{V-A} | 0 \rangle \langle V | (\bar{q} b)_{V-A} | B \rangle, \end{aligned} \quad (28)$$

with

$$\begin{aligned} a_{11} &= c_{11} + \frac{c_{12}}{N'_c}, & a_{12} &= c_{12} + \frac{c_{11}}{N'_c}, \\ a_{13} &= c_{13} + \frac{c_{12}}{N'_c}, & a_{14} &= c_{14} + \frac{c_{13}}{N'_c}, \\ a_{15} &= c_{15} + \frac{c_{16}}{N'_c}, & a_{16} &= c_{16} + \frac{c_{15}}{N'_c}, \end{aligned} \quad (29)$$

$N'_c$  is the effective color number related to the new six operators of neutral Higgs mediated processes. In this paper we fix it to be 3 when estimating the neutron Higgs effects. As for the SM operators, besides the perturbative QCD and EW corrections to the hadronic matrix elements that can be factorized into the effective Wilson coefficients, there still exist the nonfactorizable effects, such as the spectator quark effects, annihilation diagrams and spacelike penguins. Consider an arbitrary operator of the form  $O = \bar{q}_1^\alpha \Gamma q_2^\beta \bar{q}_3^\beta \Gamma' q_4^\alpha$  which arises from the Fierz transformation of a singlet-singlet operator with  $\Gamma$  and  $\Gamma'$  being some combinations of Dirac matrices. By using the identity

$$O = \frac{1}{3} \bar{q}_1 \Gamma q_2 \bar{q}_3 \Gamma' q_4 + \frac{1}{2} \bar{q}_1 \lambda^\alpha \Gamma q_2 \bar{q}_3 \lambda^\alpha \Gamma' q_4, \quad (30)$$

the matrix element  $M \rightarrow P_1 P_2$  can then be expanded as

$$\begin{aligned} \langle P_1 P_2 | O | M \rangle &= \frac{1}{3} \langle P_1 | \bar{q}_1 \Gamma q_2 | 0 \rangle \langle P_2 | \bar{q}_3 \Gamma' q_4 | M \rangle_f \\ &\quad + \frac{1}{3} \langle P_1 | \bar{q}_1 \Gamma q_2 \bar{q}_3 \Gamma' q_4 | M \rangle_{nf} \\ &\quad + \frac{1}{2} \langle P_1 P_2 | \bar{q}_1 \lambda^\alpha \Gamma q_2 \bar{q}_3 \lambda^\alpha \Gamma' q_4 | M \rangle_{nf} \end{aligned} \quad (31)$$

The last two terms on the right-hand side are nonfactorizable, and their contributions are included in the effective color number  $N_c^{\text{eff}}$ . To evaluate the decay amplitudes, it is useful to introduce the combination of Wilson coefficients

$$\begin{aligned} a_{2i}^{\text{eff}} &= c_{2i}^{\text{eff}} + \frac{1}{(N_c^{\text{eff}})_{2i}} c_{2i-1}^{\text{eff}}, \\ a_{2i-1}^{\text{eff}} &= c_{2i-1}^{\text{eff}} + \frac{1}{(N_c^{\text{eff}})_{2i-1}} c_{2i}^{\text{eff}}, \end{aligned} \quad (32)$$

The values of  $N_c^{\text{eff}}$  may be taken from Ref. [35]:

$$\begin{aligned} N_c^{\text{eff}}(V - A) &\equiv (N_c^{\text{eff}})_1 \approx (N_c^{\text{eff}})_2 \approx (N_c^{\text{eff}})_3 \approx (N_c^{\text{eff}})_4 \\ &\approx (N_c^{\text{eff}})_9 \approx (N_c^{\text{eff}})_{10}, \\ N_c^{\text{eff}}(V + A) &\equiv (N_c^{\text{eff}})_5 \approx (N_c^{\text{eff}})_6 \approx (N_c^{\text{eff}})_7 \approx (N_c^{\text{eff}})_8. \end{aligned} \quad (33)$$

According to the analysis of Ref. [35], one has in general  $N_c^{\text{eff}}(V - A) \neq N_c^{\text{eff}}(V + A)$ . In principle,  $N_c^{\text{eff}}$  can vary from channel to channel, however, in the energetic two-body  $B$  decays,  $N_c^{\text{eff}}$  is expected to be process insensitive as supported by the current data. The satisfied choice is that  $N_c^{\text{eff}}(V - A) < 3 < N_c^{\text{eff}}(V + A)$ . And it is reasonable to take the value of  $N_c^{\text{eff}}(V - A) = 2$ ,  $N_c^{\text{eff}}(V + A) = 5$ . From now on, we will drop the superscript ‘‘eff’’ through the paper for convenience.

### III. $B \rightarrow PV$ DECAYS IN TYPE III 2HDM

Based on the effective Hamiltonian obtained via the operator product expansion and renormalization group evaluation, one can write down the amplitude for  $B \rightarrow PV$  decays and calculate the branching ratios and  $CP$  violating asymmetries once a method is derived for computing the hadronic matrix elements.

We begin with the following definitions for the branching ratio and  $CP$ -violating asymmetry:

$$A_{CP} = \frac{|\bar{A}|^2 - |A|^2}{|\bar{A}|^2 + |A|^2}, \quad (34)$$

$$\text{BR}(B \rightarrow PV) = \frac{1}{2} \frac{p_c^3}{8\pi m_V^2} \tau_B (|\bar{A}|^2 + |A|^2) / (\epsilon \cdot p_B)^2,$$

where  $A$  and  $\bar{A}$  are the decay amplitudes of  $B$  and  $\bar{B}$  respectively,  $\epsilon$  is the polarization vector of the vector meson. The input parameters in our calculations are listed in Table I. The Wolfenstein parameters of the CKM matrix elements are taken to be [40]:  $A = 0.8533 \pm 0.0512$ ,  $\lambda = 0.2200 \pm 0.0026$ ,  $\bar{\rho} = 0.20 \pm 0.09$ ,  $\bar{\eta} = 0.33 \pm 0.05$ , with  $\bar{\rho} = \rho(1 - \frac{\lambda^2}{2})$ ,  $\bar{\eta} = \eta(1 - \frac{\lambda^2}{2})$ .

Here  $f_M$  and  $f_M^T$  are the decay constants of mesons.  $f_M$  can directly be determined from the experimental measurements and  $f_M^T$  could be calculated from quenched lattice QCD and QCD sum rules [41,42]. As for the form factors of pseudoscalar and vector mesons, we use the results from light-cone sum rules (LCSR) [39,43]. For the form factor involving  $\eta'$ , we use the results given by BSW [44]. Concerning the  $\eta - \eta'$  mixing effects, we take the results given in Ref. [45]. All the  $B \rightarrow P(V)$  form factors are listed in Table II and III. For comparison, we list both the results for light-cone sum rules (LCSR) in full QCD and from light-cone sum rules within the framework of heavy quark effective field theory [46].

Here  $\lambda_{ij}(i, j = c, s, b, t)$ ,  $m_{H^\pm}$ ,  $m_{h_0}$ ,  $m_{A_0}$ ,  $m_{H_0}$  are all free parameters that should be constrained from experiments. It was shown from  $B_{d,s}^0 - \bar{B}_{d,s}^0$  mixing that the parameters  $|\lambda_{cc}|$  and  $|\lambda_{ss}|$  can reach to be around 100 [24], and their phases are not constrained too much. In our present considerations, we simply fix their phases to be  $\pi/4$ . For  $\lambda_{tt}$  and  $\lambda_{bb}$ , the constraints are mainly resulted from the experimental data for the  $B - \bar{B}$  mixing,  $\Gamma(b \rightarrow s\gamma)$ ,  $\Gamma(b \rightarrow c\tau\bar{\nu}_\tau)$ ,  $\rho_0$ ,  $R_b$ , and the electric dipole moments (EDMS) of the electron and neutron [17,19,26,32,47]. For numerical calculations, we choose the following three typical parameter spaces which are allowed by the present experiments:

$$\begin{aligned} \text{case A: } & |\lambda_{tt}| = 0.15; & |\lambda_{bb}| &= 50, \\ \text{case B: } & |\lambda_{tt}| = 0.3; & |\lambda_{bb}| &= 30, \\ \text{case C: } & |\lambda_{tt}| = 0.03; & |\lambda_{bb}| &= 100, \end{aligned} \quad (35)$$

and

TABLE I. Input parameters.

$\tau_{B_d}$	$\tau_{B_s}$	$M_{B_d}$	$M_{B_s}$	$m_b$
$1.528 \times 10^{-12}$ ps	$1.472 \times 10^{-12}$ ps	5.28 GeV	5.37 GeV	4.2 GeV
$m_t$	$m_u$	$m_d$	$m_c$	$m_s$
174 GeV	3.2 MeV	6.4 MeV	1.1 GeV	0.105 GeV
$m_{\pi^\pm}$	$m_{\pi^0}$	$m_\eta$	$m_{\eta'}$	$m_{\rho^0}$
0.14 GeV	0.135 GeV	0.547 GeV	0.958 GeV	0.77 GeV
$m_{\rho^\pm}$	$m_\omega$	$m_\phi$	$m_{K^\pm}$	$m_{K^0}$
0.77 GeV	0.782 GeV	1.02 GeV	0.494 GeV	0.498 GeV
$m_{K^{*\pm}}$	$m_{K^{*0}}$	$\Lambda_{\text{QCD}}$	$f_\pi$	$f_K$
0.892 GeV	0.896 GeV	225 MeV	0.132 GeV	0.16 GeV
$f_\rho$	$f_\omega$	$f_{K^*}$	$f_\phi$	$f_\rho^T$
0.21 GeV	0.195 GeV	0.221 GeV	0.237 GeV	0.147 GeV
$f_\omega^T$	$f_{K^*}^T$	$f_\phi^T$		
0.133 GeV	0.156 GeV	0.183 GeV		

TABLE II. The relevant form factors at  $q^2 = 0$  for  $B \rightarrow P$  transitions from LCSR [39,41,43] (the first line), sum rule in heavy quark effective field theory [46] (the second line) and BSW model [44] (the third line). The values in the square brackets are the  $B \rightarrow \eta'$  form factors.

Decay channel	$B_q \rightarrow \pi$	$B_q \rightarrow K$	$B_q \rightarrow \eta^{(\prime)}$	$B_s \rightarrow K$	$B_s \rightarrow \eta^{(\prime)}$
$F_0$ LCSR	0.258	0.331	0.275[...]	...	...
SRHQEFT	0.285	0.345	0.247[...]	0.296	0.281[-]
BSW	0.333	0.379	0.307[0.254]	0.274	0.335[0.282]

$$\theta_{tt} + \theta_{bb} = \pi/2. \quad (36)$$

For the Higgs masses, the following values are assumed:

$$\begin{aligned} m_{A_0} &\simeq 120 \text{ GeV}, & m_{h_0} &\simeq 115 \text{ GeV}, \\ m_{H_0} &\simeq 160 \text{ GeV}, & m_{H^\pm} &\simeq 200 \text{ GeV}. \end{aligned} \quad (37)$$

The charged Higgs mediated one loop FCNC effects to the  $\Delta B = 1$  charmless decays are mostly characterized through the Wilson coefficient  $C_g^{\text{eff}}$ , which is included in the  $C_{(3,4,5,6,7,8)}^{\text{eff}}$ . Their numerical results in SM and type III 2HDM are listed in Table IV in Appendix A, from which we can see that new physics effects are very small. However, the neutral Higgs mediated processes will bring in new operators  $\mathcal{Q}_{(11,12,\dots,16)}$  with the new Wilson coefficients  $C_{(11,12,\dots,16)}$ . These coefficients may be large when

TABLE III. The relevant form factors at  $q^2 = 0$  for  $B \rightarrow V$  transitions from LCSR [39,41,43] (the first line), sum rule in heavy quark effective field theory [46] (the second line) and BSW model [44] (the third line).

Decay channel	$B_q \rightarrow \rho$	$B_q \rightarrow \omega$	$B_q \rightarrow K^*$	$B_s \rightarrow \phi$	$B_s \rightarrow K^*$
$A_0$ LCSR	0.303	0.281	0.374	0.474	0.363
SRHQEFT	0.363	0.341	0.400	0.397	0.337
BSW	0.281	0.280	0.321	0.475	0.364

the neutral Higgs bosons couple to the second and third generations of quarks. The numerical results for three parameter sets are presented in Table V in Appendix A. All the branch ratios and  $CP$  violation results in the SM and type III 2HDM are listed in Table VI, VII, VIII, and IX in Appendix B. The main theoretical uncertainty comes from the CKM matrix elements. For simplicity, we just list the possible errors in the SM calculations, similar uncertainties can be taken into account in the type III 2HDM, while large uncertainties may be caused mainly from the big parameter space of type III 2HDM.

#### IV. CONCLUSIONS AND DISCUSSIONS

From the numerical results, it is seen that in some decay channels, the new physics contributions can be significant, especially to  $CP$  violations. Firstly, let us check the  $B_d^0 \rightarrow PV$  decays. (i), as we have set the Yukawa couplings  $\lambda_{iu}$  and  $\lambda_{id}$  to be zero, the neutral Higgs contributions to  $B \rightarrow (\rho, \omega, K^*)\pi, (\rho, \omega)K$  decays can actually be ignored, only the charged Higgs provides additional new contributions. This is the reason why the branching ratio of  $B \rightarrow \bar{K}^0 \rho^0$  decay in type III 2HDM is the same as the SM prediction (about  $1.55 \times 10^{-6}$ ), which is far below the large central value of experimental data  $(5.4 \pm 0.9) \times 10^{-6}$ . Even taking the annihilation diagram and exchange diagram into account, their contributions are still not big enough to give such an enhancement. The same situation also occurs in the

$B \rightarrow K^- \rho^+$ ,  $K^{*-} \pi^+$  decays, where the experimental results are much larger than the theoretical predictions both in SM and type III 2HDM when using the generalized factorization approach. Though the branching ratios can be enhanced by using improved QCD factorization (QCDF) [48], the resulting values are still smaller than the data. (ii), note that the type III 2HDM prediction for  $CP$  violation in the  $B_d \rightarrow K \phi$  decay is 5 ~ 7 times larger than the SM prediction, which can be a signal to look for new physics in future experiments. The predictions for the branching ratios in both SM and type III 2HDM are smaller than the experimental ones. (iii), the SM and type III 2HDM predictions for branching ratio of the  $B_d \rightarrow K^{*0} \pi^0$  decay are the same in size and all consistent with the experimental data within  $1\sigma$  error. However, the new physics contribution to  $CP$  violation changes the sign of  $CP$  violation in comparison with the SM prediction, and the magnitude can be 1 ~ 5 times larger than the SM prediction, while the prediction is still consistent with the current experimental data due to extremely large errors in experiment. (iv), in the  $B_d \rightarrow K^*(\eta, \eta')$  decays, new physics effects on  $CP$  violation also become significant. In the  $B \rightarrow K^* \eta$  decay, the type III 2HDM prediction for  $CP$  violation can be negative which is opposite to the SM prediction. As for  $B \rightarrow K^* \eta'$  decay, the type III 2HDM prediction for  $CP$  violation can be as large as about 40%, which is larger by a factor of 7 to the SM estimation. (v) in the  $B_d \rightarrow \rho^0 \pi^0$  decay channel, both SM and type III 2HDM predictions for the branching ratio are much smaller than the experimental data. Such an inconsistency cannot be improved even in QCD factorization approach [48]. As for the  $CP$  violation, the SM and type III 2HDM predictions have opposite sign. Because of large errors in the current experiment data, one cannot exclude new physics effects at present stage. (vi), in the  $B_d \rightarrow \omega \pi$  decays, the new physics effects on  $CP$  violation is found to be significant, its numerical result is about -12% which may be compare with the SM prediction 5%.

For the  $B_s^0 \rightarrow PV$  decays, the new physics contributions can be large in some decay channels too. (i) in the  $B_s \rightarrow K^* \eta$  decay, the contributions from the type III 2HDM can enhance the direct  $CP$  violation to be about -50% in comparison with the SM prediction -28.8%. In contrast, for the  $B_s \rightarrow K^* \eta'$  decay, the new physics contribution reduces the  $CP$  violation from the SM result around -37% to the type III 2HDM result around -20%. (ii) in the  $B_s \rightarrow \rho \eta^{(\prime)}$  decay, new physics contributions to the branching ratio are destructive, but provide an enhancement to  $CP$  violation with a factor of 4 larger than the SM prediction. (iii), in the  $B_s \rightarrow \phi \eta^{(\prime)}$  decay, new physics effects to both branching ratios and  $CP$  violation become significant. (iv), in the  $B_s \rightarrow K^0 \phi$  decay channel, nonzero  $CP$  violation can be an evidence for new physics. This is because the SM prediction almost vanishes, but the new physics contribution in the type III 2HDM can be as large as about -10%.

In the  $B_u \rightarrow PV$  decays, there are also some interesting new effects. (i), in the  $B_u \rightarrow \pi^- \bar{K}^{*0}$  decay, the type III 2HDM prediction for  $CP$  violation can be larger by an order of magnitude in comparison with the SM prediction and is actually much closer to the experimental data. (ii), in the  $B_u \rightarrow K^- \phi$  decay,  $CP$  violation can reach to be 10% in the type III 2HDM, which is much larger than the SM prediction 1.44% and is compatible with the experimental data at  $2\sigma$  level. (iii) in the  $B_u \rightarrow K^{*-} \eta$  decay, new physics prediction for  $CP$  violation is smaller than the SM prediction but is much consistent with the experimental data. (iv) for the  $B_u \rightarrow \rho^- \eta$  decay, the type III 2HDM prediction for  $CP$  violation can be 2 ~ 3 times larger than the SM prediction and is actually closer to the experimental central value. (v), in the  $B_u \rightarrow \pi^- \phi$  decay, new physics influences on both the branching ratio and direct  $CP$  violation can become significant. (vi), in the  $B_u \rightarrow K^{*-} K^0$  decay process, the type III 2HDM prediction for  $CP$  violation can be around 20 ~ 24%, which is much larger than the SM prediction -1.73%. On the contrary, in the  $B_u \rightarrow K^{*0} K^-$  decay, the type III 2HDM prediction for  $CP$  violation may become much smaller than the SM prediction.

From the above analyzes and numerical results, it is clear that in some decay channels, the theoretical predictions for branching ratios are still far from the experimental data in both the SM and the type III 2HDM, such as  $B \rightarrow K \rho$ ,  $K^* \pi$  decays etc. Even employing the improved QCDF, the situation cannot be improved much. One should explore some new mechanism to improve those discrepancies. For simplicity, in this paper, we do not consider the possible effects caused by the final state interactions (FSI) and the possible contributions from annihilation and exchange diagrams although they may play a significant rule in some decay channels. In our numerical calculations, we have only considered three possible parameter spaces for the type III 2HDM. Also we have totally neglected the first generation Yukawa couplings and the off-diagonal matrix elements of the Yukawa coupling matrix, such as  $\lambda_{tc, sb}$ , etc. to eliminate the FCNC at tree level. However, it is still possible that FCNC involving the third generation quarks exists at tree level, so the constraints can be less stronger, for example, considering the nonzero off-diagonal elements.

In conclusion, we have shown that the new Higgs bosons in the type III 2HDM with spontaneous  $CP$  violation can bring out some significant effects in some charmless  $B$ -meson decays, which can be good signals to test the SM and to explore new physics from more precise measurements in the future  $B$  factory experiments.

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**APPENDIX A: THE EFFECTIVE WILSON COEFFICIENTS**TABLE IV. The effective Wilson coefficients  $C_{(1,2\dots 10)}^{\text{eff}}$  in  $b \rightarrow s$  process in SM and type III 2HDM at  $\mu = m_b = 4.2$  GeV.

Model	SM	Case A	Case B	Case C
$C_1^{\text{eff}}$	1.17	1.17	1.17	1.17
$C_2^{\text{eff}}$	-0.37	-0.37	-0.37	-0.37
$C_3^{\text{eff}}$	$0.024 + 0.0035I$	$0.024 + 0.006I$	$0.024 + 0.0048I$	$0.024 + 0.0075I$
$C_4^{\text{eff}}$	$-0.050 - 0.010I$	$-0.05 - 0.018I$	$-0.05 - 0.014I$	$-0.05 - 0.023I$
$C_5^{\text{eff}}$	$0.015 + 0.0035I$	$0.015 + 0.006I$	$0.015 + 0.005I$	$0.015 + 0.0075I$
$C_6^{\text{eff}}$	$-0.064 - 0.010I$	$-0.064 - 0.018I$	$-0.064 - 0.014I$	$-0.064 - 0.023I$
$C_7^{\text{eff}}$	$-0.00028 - 0.00024I$	$-0.00035 - 0.00024I$	$-0.00035 - 0.00024I$	$-0.00035 - 0.00024I$
$C_8^{\text{eff}}$	0.00055	0.00061	0.00061	0.0006
$C_9^{\text{eff}}$	$-0.011 - 0.00024I$	$-0.011 - 0.00024I$	$-0.011 - 0.00024I$	$-0.011 - 0.00024I$
$C_{10}^{\text{eff}}$	0.0038	0.00334	0.0034	0.0034

TABLE V. The Wilson coefficients  $C_{(11,12\dots 16)}^{\text{eff}}$  at  $\mu = m_b = 4.2$  GeV.

Parameter space	Case A	Case B	Case C
$C_{11}^c$	$-0.089 + 0.12I$	$-0.089 + 0.19I$	$-0.11 + 0.13I$
$C_{12}^c$	0	0	0
$C_{13}^c$	$-0.031 - 0.051I$	$-0.054 - 0.072I$	$-0.030 - 0.055I$
$C_{14}^c$	$-0.00063 - 0.0010I$	$-0.0011 - 0.0015I$	$-0.00061 - 0.0011I$
$C_{15}^c$	$0.00035 + 0.00057I$	$0.00061 + 0.00080I$	$0.00034 + 0.00062I$
$C_{16}^c$	$-0.0011 - 0.00175I$	$-0.0019 - 0.0025I$	$-0.0010 - 0.0019I$
$C_{11}^s$	$-0.0085 + 0.012I$	$-0.0085 + 0.018I$	$-0.010 + 0.012I$
$C_{12}^s$	0	0	0
$C_{13}^s$	$-0.0030 - 0.0049I$	$-0.0052 - 0.0069I$	$-0.0029 - 0.0052I$
$C_{14}^s$	$-0.000060 - 0.00010I$	$-0.00011 - 0.00014I$	$-0.000059 - 0.00010I$
$C_{15}^s$	$0.000033 + 0.000055I$	$0.000058 + 0.000078I$	$0.000032 + 0.000059I$
$C_{16}^s$	$-0.00010 - 0.00017I$	$-0.00018 - 0.00024I$	$-0.0001 - 0.00018I$

**APPENDIX B: NUMERICAL RESULTS OF  $B \rightarrow PV$  DECAYS**

TABLE VI.  $CP$  averaged branching ratios (in units of  $10^{-6}$ ) (first line) and direct  $CP$  violation (second line) for charmless  $B_d^0 \rightarrow PV$  decays in SM and type III 2HDM.  $N_c^{\text{eff}}(V-A)$ ,  $N_c^{\text{eff}}(V+A)$  are fixed to be 2 and 5, respectively, and  $N_c' = 3$ . The parameter spaces are: case A: ( $|\lambda_{tt}| = 0.15$ ,  $|\lambda_{bb}| = 50$ ,  $\theta = \pi/2$ ), case B: ( $|\lambda_{tt}| = 0.03$ ,  $|\lambda_{bb}| = 100$ ,  $\theta = \pi/2$ ), case C: ( $|\lambda_{tt}| = 0.3$ ,  $|\lambda_{bb}| = 30$ ,  $\theta = \pi/2$ ), and  $\lambda_{cc} = \lambda_{ss} = 100e^{i\pi/4}$ .

Decay channel	SM	Case A (2HDM)	Case B (2HDM)	Case C (2HDM)	Exp
$B_d^0 \rightarrow K^0 \rho^0$	$1.56^{+0.48}_{-0.24}$ ( $1.7^{+0.40}_{-0.20}$ )%	1.55 2.10%	1.55 1.97%	1.56 2.20%	$5.4 \pm 0.9$ ...
$B_d^0 \rightarrow K^- \rho^+$	$2.01^{+0.75}_{-0.58}$ ( $-3.6^{+0.90}_{-1.10}$ )%	1.94 -3.83%	1.97 -3.90%	1.91 -3.76%	$9.9^{+1.6}_{-1.5}$ ( $17^{+15}_{-16}$ )%
$B_d^0 \rightarrow K^{*0} \pi^+$	$3.24^{+1.46}_{-0.82}$ ( $24.5^{+7.0}_{-5.8}$ )%	3.92 27.5%	3.56 26.2%	4.33 28.2%	$9.8 \pm 1.1$ ( $-5 \pm 14$ )%
$B_d^0 \rightarrow K^{*0} \pi^0$	$1.47^{+0.38}_{-0.19}$ ( $-2.50^{+0.60}_{-0.70}$ )%	1.47 7.20%	1.46 2.30%	1.51 11.5%	$1.7 \pm 0.8$ ( $-1^{+27}_{-26}$ )%
$B_d^0 \rightarrow K^0 \phi$	$4.80^{+1.11}_{-0.52}$ ( $1.40^{+0.00}_{-0.00}$ )%	5.22 5.96%	5.23 10.0%	5.18 10.3%	$8.3^{+1.2}_{-1.0}$ ...
$B_d^0 \rightarrow K^* \eta$	$9.41^{+1.1}_{-0.96}$ ( $1.86^{+0.20}_{-0.10}$ )%	10.4 -2.68%	10.7 -3.85%	10.8 -1.93%	$16.1 \pm 1.0$ ( $19 \pm 5$ )%
$B_d^0 \rightarrow K^* \eta'$	$1.33^{+0.21}_{-0.17}$ ( $5.50^{+0.80}_{-0.60}$ )%	1.18 32.7%	1.49 22.1%	1.20 40.4%	$3.8 \pm 1.2$ ( $-8 \pm 25$ )%
$B_d^0 \rightarrow K^0 \omega$	$0.43^{+0.17}_{-0.08}$ ( $0.00^{+0.01}_{-0.01}$ )%	0.44 0.33%	0.44 0.32%	0.44 0.32%	$4.8 \pm 0.6$ ...
$B_d^0 \rightarrow \rho^- \pi^+$	$15.8^{+6.43}_{-5.82}$ ( $-4.3^{+1.00}_{-1.30}$ )%	15.3 -4.4%	15.1 -4.3%	15.1 -4.4%	$24.0 \pm 2.5$ ...

TABLE VII. Continue Table VI.

Decay channel	SM	Case A (2HDM)	Case B (2HDM)	Case C (2HDM)	Exp
$B_d^0 \rightarrow \rho^+ \pi^-$	$17.3^{+2.34}_{-1.86}$ ( $-18.8^{+2.30}_{-1.30}$ )%	16.3 -26.5%	17.7 -26.4%	15.0 -26.4%	$24.0 \pm 2.5$ -
$B_d^0 \rightarrow K^{0*} \bar{K}^0$	$0.23^{+0.11}_{-0.06}$ ( $-11.5^{+5.40}_{-3.71}$ )%	0.24 -10.1%	0.24 -14.6%	0.25 -6.45%	$<1.9$ ...
$B_d^0 \rightarrow K^0 \bar{K}^{*0}$	$0.038^{+0.01}_{-0.01}$ ( $-1.73^{+0.09}_{-0.11}$ )%	0.037 20.3%	0.036 22.0%	0.037 24.3%	... ...
$B_d^0 \rightarrow \phi \eta$	$0.0039^{+0.00}_{-0.00}$ ( $1.13^{+0.23}_{-0.23}$ )%	0.0038 1.35%	0.0038 1.25%	0.0038 1.45%	$<0.6$ ...
$B_d^0 \rightarrow \phi \eta'$	$0.0023^{+0.00}_{-0.00}$ ( $1.13^{+0.23}_{-0.23}$ )%	0.0022 1.35%	0.0024 1.25%	0.0022 1.45%	$<1.0$ ...
$B_d^0 \rightarrow \phi \pi$	$0.015^{+0.00}_{-0.01}$ ( $3.90^{+0.00}_{-0.00}$ )%	0.0017 1.35%	0.0017 1.25%	0.0016 1.45%	$<0.28$ ...
$B_d^0 \rightarrow \rho^0 \pi^0$	$0.80^{+0.55}_{-0.43}$ ( $-10.5^{+1.20}_{-1.30}$ )%	0.81 14.4%	0.82 13.7%	0.80 14.9%	$1.8^{+0.6}_{-0.5}$ ( $-49^{+70}_{-83}$ )%
$B_d^0 \rightarrow \rho \eta$	$0.82^{+0.55}_{-0.25}$ ( $12.3^{+2.30}_{-2.51}$ )%	0.88 6.93%	0.83 3.21%	0.92 6.91%	$<1.5$ ...
$B_d^0 \rightarrow \rho \eta'$	$0.50^{+0.33}_{-0.17}$ ( $5.88^{+1.21}_{-1.20}$ )%	0.55 6.33%	0.54 6.87%	0.57 6.20%	$<3.7$ ...
$B_d^0 \rightarrow \omega \pi$	$0.60^{+0.34}_{-0.17}$ ( $-4.97^{+1.10}_{-1.22}$ )%	0.56 12.4%	0.53 12.7%	0.59 12.1%	$<1.2$ ...
$B_d^0 \rightarrow \omega \eta$	$0.84^{+0.58}_{-0.30}$ ( $-13.9^{+2.90}_{-4.32}$ )%	0.77 -11.1%	0.80 -9.04%	0.73 -11.2%	$<1.9$ ...
$B_d^0 \rightarrow \omega \eta'$	$0.53^{+0.34}_{-0.20}$ ( $-19.7^{+3.90}_{-6.00}$ )%	0.46 -25.0%	0.50 -26.0%	0.44 -26.1%	$<2.8$ ...

TABLE VIII.  $CP$  averaged branching ratios (in units of  $10^{-6}$ ) (first line) and direct  $CP$  violation (second line) for charmless  $B_s^0 \rightarrow PV$  decays in SM and type III 2HDM.

Decay channel	SM	Case A (2HDM)	Case B (2HDM)	Case C (2HDM)
$B_s^0 \rightarrow K^{*+} \pi^-$	$8.34^{+5.70}_{-3.37}$ $(-0.13^{+0.00}_{-0.00})\%$	8.73 -0.12%	8.34 -0.13%	8.44 -0.13%
$B_s^0 \rightarrow K^+ \rho^-$	$26.7^{+9.42}_{-9.75}$ $(-4.3^{+0.90}_{-1.30})\%$	27.7 -4.3%	26.5 -4.3%	26.2 -4.4%
$B_s^0 \rightarrow K^{*0} \pi^0$	$0.21^{+0.14}_{-0.09}$ $(5.0^{+0.80}_{-1.11})\%$	0.20 5.1%	0.21 5.1%	0.21 5.1%
$B_s^0 \rightarrow \rho K^0$	$0.59^{+0.35}_{-0.21}$ $(16.5^{+3.01}_{-3.10})\%$	0.70 14.2%	0.66 14.7%	0.73 13.6%
$B_s^0 \rightarrow K^0 \omega$	$0.70^{+0.40}_{-0.23}$ $(-18.3^{+3.80}_{-5.00})\%$	0.73 -18.3%	0.69 -18.4%	0.68 -18.1%
$B_s^0 \rightarrow K^* \eta$	$0.29^{+0.12}_{-0.07}$ $(-28.8^{+5.70}_{-6.31})\%$	0.32 -43.2%	0.31 -49.9%	0.33 -42.8%
$B_s^0 \rightarrow K^* \eta'$	$0.20^{+0.07}_{-0.04}$ $(-37.1^{+6.51}_{-7.31})\%$	0.23 -21.2%	0.21 -21.3%	0.25 -17.7%
$B_s^0 \rightarrow K^- K^{*+}$	$1.98^{+0.63}_{-0.32}$ $(-3.6^{+1.35}_{-1.24})\%$	2.27 -3.3%	2.24 -3.4%	2.31 -3.2%
$B_s^0 \rightarrow K^+ K^{*-}$	$5.49^{+1.25}_{-1.41}$ $(24.5^{+5.21}_{-3.80})\%$	6.97 22.8%	6.81 20.3%	7.02 21.6%
$B_s^0 \rightarrow \rho \eta$	$0.21^{+0.09}_{-0.04}$ $(3.6^{+0.80}_{-0.80})\%$	0.04 18.4%	0.04 18.4%	0.04 18.3%
$B_s^0 \rightarrow \rho \eta'$	$0.12^{+0.06}_{-0.02}$ $(3.6^{+0.90}_{-0.80})\%$	0.03 18.3%	0.02 18.4%	0.03 18.4%
$B_s^0 \rightarrow \phi \pi$	$0.21^{+0.08}_{-0.05}$ $(0.00^{+0.00}_{-0.00})\%$	0.04 0.00	0.03 0.00	0.04 0.00
$B_s^0 \rightarrow \omega \eta$	$0.02^{+0.01}_{-0.01}$ $(43.1^{+10.00}_{-8.50})\%$	0.02 40.0%	0.02 39.6%	0.02 40.1%
$B_s^0 \rightarrow \omega \eta'$	$0.01^{+0.01}_{-0.00}$ $(43.1^{+9.80}_{-8.11})\%$	0.01 40.0%	0.01 39.6%	0.01 40.1%
$B_s^0 \rightarrow \phi \eta$	$12.2^{+2.73}_{-1.24}$ $(2.2^{+0.20}_{-0.20})\%$	17.9 -12.3%	17.7 -10.6%	20.0 -14.2%
$B_s^0 \rightarrow \phi \eta'$	$0.61^{+0.11}_{-0.06}$ $(15.6^{+3.30}_{-2.50})\%$	1.68 -21.2%	1.92 -21.3%	2.23 -17.7%
$B_s^0 \rightarrow K^0 \bar{K}^{*}$	$5.78^{+1.38}_{-0.6}$ $(1.27^{+0.54}_{-0.32})\%$	8.03 4.10%	7.00 2.29%	9.14 5.0%
$B_s^0 \rightarrow K^{*0} \bar{K}$	$1.28^{+0.50}_{-0.39}$ $(1.0^{+0.21}_{-0.10})\%$	1.03 1.2%	1.00 2.2%	1.06 1.0%
$B_s^0 \rightarrow \phi K^0$	$0.14^{+0.07}_{-0.04}$ $(0.23^{+0.00}_{-0.00})\%$	0.12 -9.7%	0.12 -8.8%	0.12 -11.7%

TABLE IX.  $CP$  averaged branching ratios (in units of  $10^{-6}$ ) (first line) and direct  $CP$  violation (second line) for charmless  $B_u^- \rightarrow PV$  decays in SM and type III 2HDM.

Decay channel	SM	Case A 2HDM)	Case B (2HDM)	Case C (2HDM)	Exp.
$B_u^- \rightarrow K^- \rho^0$	$0.59^{+0.40}_{-0.22}$ $(-1.88^{+0.50}_{-0.70})\%$	0.58 -2.40%	0.58 -2.32%	0.56 -2.38%	$4.25^{+0.55}_{-0.56}$ $(31^{+11}_{-10})\%$
$B_u^- \rightarrow K^{*-} \pi^0$	$2.62^{+1.22}_{-0.73}$ $(18.9^{+5.10}_{-4.44})\%$	2.80 22.3%	3.25 20.4%	2.80 22.3%	$6.9 \pm 2.3$ $(4 \pm 29)\%$
$B_u^- \rightarrow \bar{K}^0 \rho^-$	$1.09^{+0.26}_{-0.11}$ $(0.34^{+0.00}_{-0.00})\%$	1.10 1.15%	1.10 0.75%	1.10 1.15%	<48 ...
$B_u^- \rightarrow \pi^- \bar{K}^{*0}$	$3.67^{+0.87}_{-0.39}$ $(-1.28^{+1.60}_{-1.60})\%$	3.88 -12.9%	3.66 -5.41%	3.88 -12.9%	$11.3 \pm 1.0$ $(-8.6 \pm 5.6)\%$
$B_u^- \rightarrow K^- \omega$	$2.22^{+0.35}_{-0.48}$ $(0.00^{+0.00}_{-0.00})\%$	2.17 -0.33%	2.20 -0.32%	2.17 -0.33%	$6.9 \pm 0.5$ $(5 \pm 6)\%$
$B_u^- \rightarrow K^- \phi$	$5.16^{+1.18}_{-0.52}$ $(1.44^{+0.01}_{-0.01})\%$	5.92 11.7%	5.57 10.0%	5.93 10.3%	$8.30 \pm 0.65$ $(3.4 \pm 4.4)\%$
$B_u^- \rightarrow K^{*-} \eta$	$9.36^{+2.83}_{-1.59}$ $(13.6^{+3.71}_{-3.00})\%$	10.51 6.73%	11.09 10.2%	10.6 4.52%	$19.5^{+1.6}_{-1.5}$ $(2 \pm 6)\%$
$B_u^- \rightarrow K^{*-} \eta'$	$1.53^{+0.78}_{-0.46}$ $(52.2^{+12.80}_{-11.90})\%$	1.32 55.4%	1.38 52.4%	1.37 56.9%	$4.9^{+2.1}_{-1.9}$ $(30^{+33}_{-37})\%$
$B_u^- \rightarrow \pi^0 \rho^-$	$11.4^{+3.96}_{-3.05}$ $(-3.0^{+0.61}_{-1.00})\%$	11.1 -3.1%	11.3 -3.0%	11.1 -3.1%	$10.8^{+1.4}_{-1.5}$ $(2 \pm 11)\%$
$B_u^- \rightarrow \pi^- \rho^0$	$7.36^{+3.14}_{-2.36}$ $(4.2^{+1.1}_{-0.8})\%$	7.75 4.1%	7.50 4.2%	7.75 4.1%	$8.7^{+1.0}_{-1.1}$ $(-7^{+12}_{-13})\%$
$B_u^- \rightarrow \pi^- \omega$	$6.85^{+2.66}_{-2.54}$ $(-4.7^{+1.00}_{-1.40})\%$	6.50 -4.8%	6.65 -4.7%	6.50 -4.8%	$6.7 \pm 0.6$ $(-4 \pm 7)\%$
$B_u^- \rightarrow \rho^- \eta$	$11.1^{+3.58}_{-2.74}$ $(-0.90^{+0.33}_{-0.40})\%$	13.2 -2.35%	11.0 -3.34%	10.8 -2.36%	$5.3^{+1.2}_{-1.1}$ $(1 \pm 16)\%$
$B_u^- \rightarrow \rho^- \eta'$	$14.0^{+3.26}_{-2.24}$ $(-9.9^{+2.10}_{-2.90})\%$	12.7 -10.1%	13.7 -9.60%	12.8 -10.1%	$9.1^{+3.7}_{-2.8}$ $(-4 \pm 28)\%$
$B_u^- \rightarrow \pi^- \phi$	$0.0036^{+0.00}_{-0.00}$ $(1.13^{+0.00}_{-0.00})\%$	0.016 15.5%	0.016 7.96%	0.016 15.5%	<0.24 ...
$B_u^- \rightarrow K^{*-} K^0$	$0.038^{+0.02}_{-0.01}$ $(-1.73^{+0.00}_{-0.00})\%$	0.037 20.3%	0.036 22.0%	0.037 24.3%	... ...
$B_u^- \rightarrow K^- K^{*0}$	$0.25^{+0.12}_{-0.06}$ $(-37.1^{+11.61}_{-9.21})\%$	0.27 -5.13%	0.26 -14.6%	0.27 -6.45%	<5.3 ...

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