Reinvestigating the $B \to PP$ decays by including the contributions from $\phi_{B2}$

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Abstract

Considering the $B$ mesonic distribution amplitude $\phi_{B2}$, we reinvestigated the $B \to PP$ (where $P = \pi$ and $K$) decays with the perturbative QCD (pQCD) approach based on the $k_T$ factorization for three scenarios. It is found that the contributions of $\phi_{B2}$ to formfactors $F_0^{B\to P(0)}$ and branching ratios are comparable with those from the NLO corrections. The $B \to K\pi$ decays could be well explained by considering the $\phi_{B2}$. Hence, when the nonleptonic $B$ decays are studied with the pQCD approach, the $\phi_{B2}$ should be taken into account seriously.
It is well known that many breakthrough discoveries have come from precise experiments. B physics is on the bleeding edge and one of hot topics of current particle physics, because of the renewed impetus from the successive CLEO, BaBar, Belle, LHCb and Belle-II experiments. Various B meson decay modes with branching ratio larger than $10^{-6}$ have been extensively studied by the BaBar and Belle Collaborations with $0.56 \text{ ab}^{-1}$ and $1.02 \text{ ab}^{-1}$ data samples in the past years [1, 2]. A few phenomena of inconsistencies between experimental measurements and theoretical expectations from the standard model (SM) are emerging. More and more B meson data are expected in the near future, about $50 \text{ ab}^{-1}$ by the Belle-II detector at the $e^+e^-$ SuperKEKB collider [3] and about $300 \text{ fb}^{-1}$ by the LHCb detector at the High Luminosity LHC (HL-LHC) hadron collider [4]. Besides some new phenomena, the much more precise measurements of B meson weak decays will offer a much more rigorous test on SM. When looking for a smoking gun of new physics and settling the temporary differences between experimental and theoretical results, a more careful calculation on B meson decays within SM is very necessary and important. In this paper, we will reinvestigate the $B \to PP$ decays (here $P = \pi$ and $K$) based on the perturbative QCD approach within SM, by considering the contributions from B mesonic wave function $\phi_{B2}$ which usually attract less attention in previous calculation.

For clarity, we will sketch the phenomenological study of nonleptonic $B \to PP$ decays, although they have been extensively studied, for example, in Refs. [5–13]. Because of our inadequate comprehension of the flavor mixing and possible glueball components, the final states of $\eta$ and $\eta'$ mesons are not considered here for the moment.

At the quark level, based on the operator product expansion and renormalization group (RG) method, the effective Hamiltonian responsible for $B \to PP$ decays is written as [14],

$$\mathcal{H}_{\text{eff}} = \frac{G_F}{\sqrt{2}} \sum_{q=d,s} \left\{ V_{ub} V_{ud}^* \sum_{i=1}^{2} C_i Q_i - V_{tb} V_{td}^* \sum_{j=3}^{10} C_j O_j \right\} + \text{h.c.}, \quad (1)$$

where $G_F \simeq 1.166 \times 10^{-5} \text{ GeV}^{-2}$ [1] is the Fermi weak coupling constant. With the Wolfenstein parametrization, the related Cabibbo-Kobayashi-Maskawa (CKM) factors are written as follows.

$$V_{ub} V_{ud}^* = A \lambda^3 (\rho - i \eta) \left(1 - \frac{1}{2} \lambda^2 - \frac{1}{8} \lambda^4\right) + \mathcal{O}(\lambda^8), \quad (2)$$

$$V_{tb} V_{td}^* = A \lambda^3 + A^3 \lambda^7 (\rho - i \eta - \frac{1}{2}) - V_{ub} V_{ud}^* + \mathcal{O}(\lambda^8), \quad (3)$$

$$V_{ub} V_{us}^* = A \lambda^3 (\rho - i \eta) + \mathcal{O}(\lambda^8), \quad (4)$$
\[ V_{tb} V_{ts}^* = -A \lambda^2 (1 - \frac{1}{2} \lambda^2 - \frac{1}{8} \lambda^4) + \frac{1}{2} A^3 \lambda^6 - V_{ub} V_{us}^* + \mathcal{O}(\lambda^8), \]  

and the latest values of the four Wolfenstein parameters \((A, \lambda, \rho \text{ and } \eta)\) from data with the CKMfitter method \([1]\) are listed in Table I. The Wilson coefficients, \(C_i\), are perturbatively calculable at the scale of \(\mathcal{O}(m_W)\) and then evolved to the \(b\) quark decay scale \(\mathcal{O}(m_b)\) with the RG equation \([14]\). The combinations of the well determined \(G_F,\) CKM factors and \(C_i\) could be regarded as the universal and effective couplings of the operators \(O_i\). The tree operators \(O_{1,2}\), QCD penguin operators \(O_{3-6}\) and electromagnetic penguin operators \(O_{7-10}\) are local four-quark interactions and expressed as follows.

\[
O_1 = (\bar{u}_a b_a)_{V-A}(\bar{q}_\beta u_\beta)_{V-A}, \\
O_2 = (\bar{u}_a b_\beta)_{V-A}(\bar{q}_\beta u_\alpha)_{V-A}, \\
O_3 = (\bar{q}_\alpha b_\alpha)_{V-A} \sum_{q'} (\bar{q}'_\beta q'_\beta)_{V-A}, \\
O_4 = (\bar{q}_\alpha b_\beta)_{V-A} \sum_{q'} (\bar{q}'_\beta q'_\alpha)_{V-A}, \\
O_5 = (\bar{q}_\alpha b_\alpha)_{V-A} \sum_{q'} (\bar{q}'_\beta q'_\alpha)_{V+A}, \\
O_6 = (\bar{q}_\alpha b_\beta)_{V-A} \sum_{q'} (\bar{q}'_\beta q'_\alpha)_{V+A}, \\
O_7 = (\bar{q}_\alpha b_\alpha)_{V-A} \sum_{q'} \frac{3}{2} Q_{q'} (\bar{q}'_\beta q'_\beta)_{V+A}, \\
O_8 = (\bar{q}_\alpha b_\beta)_{V-A} \sum_{q'} \frac{3}{2} Q_{q'} (\bar{q}'_\beta q'_\alpha)_{V+A}, \\
O_9 = (\bar{q}_\alpha b_\alpha)_{V-A} \sum_{q'} \frac{3}{2} Q_{q'} (\bar{q}'_\beta q'_\alpha)_{V-A}, \\
O_{10} = (\bar{q}_\alpha b_\beta)_{V-A} \sum_{q'} \frac{3}{2} Q_{q'} (\bar{q}'_\beta q'_\alpha)_{V-A},
\]

where \((\bar{q}_1 q_2)_{V_A} \equiv \bar{q}_1 \gamma^\mu (1 \pm \gamma_5) q_2; \alpha \text{ and } \beta \text{ is the color indices; } Q_{q'} \text{ is the electric charge of quark } q' \text{ in the unit of } |e|;\) and \(q' \in \{u, d, c, s, b\}\).

The hadronic matrix elements (HMEs), \(\langle O_i \rangle \equiv \langle P_1 P_2 | O_i | B \rangle\), describe the transformations from the quarks to hadrons. The calculation of HMEs is on the one hand very complicated due to the entanglements between perturbative and nonperturbative contributions, and on the other hand very sensitive to phenomenological models because of our limited knowledge of dynamics of hadronization and final state interactions. One of the main challenges
is to calculate HMEs as properly as possible. Theoretically, the radiative corrections to HMEs should be appropriately included so that the strong phase angles closely related to CP violation could be obtained. For nonleptonic $B$ decays, the HMEs are usually written as the product of the rescattering amplitudes of quarks (which are calculable order by order with perturbation theory in principle) and wave functions of participating hadrons (where nonperturbative contributions are housed) with the fashionable QCD-inspired phenomenological models, either the QCD factorization (QCDF) approach [15–20] based on the collinear approximation or the perturbative QCD (pQCD) approach [21–27] retaining the effects of transverse momentum $k_T$. Hadronic wave functions (WFs) or distribution amplitudes (DAs) are independent of specific process and determined from data, which enable evaluating HMEs to simplify greatly.

WFs and/or DAs are the essential ingredients of the master formulas for evaluating HMEs with the QCDF and pQCD approaches. The $B$ mesonic WFs are generally composed of two scalar functions [28, 29] and written as follows with the convention of Refs. [30, 31].

$$
\langle 0 | \bar{q}_{\alpha}(z) b_{\beta}(0) | \mathcal{F}(p) \rangle = + \frac{i}{4} f_B \int d^4 k e^{-i k \cdot z} \left\{ \left( \hat{\varphi}_{\alpha} + m_B \right) \gamma_5 \left[ \frac{\hat{f}_B^+}{\sqrt{2}} \varphi_B^+ + \frac{\hat{f}_B^-}{\sqrt{2}} \varphi_B^- \right] \right\}_{\beta \alpha} = - \frac{i}{4} f_B \int d^4 k e^{-i k \cdot z} \left\{ \left( \hat{\varphi}_{\alpha} + m_B \right) \gamma_5 \left[ \varphi_B^+ + \frac{\hat{f}_B^-}{\sqrt{2}} \left( \phi_B^+ - \phi_B^- \right) \right] \right\}_{\beta \alpha} = - \frac{i}{4} f_B \int d^4 k e^{-i k \cdot z} \left\{ \left( \hat{\varphi}_{\alpha} + m_B \right) \gamma_5 \left( \phi_{B1} + \frac{\hat{f}_B^-}{\sqrt{2}} \phi_{B2} \right) \right\}_{\beta \alpha},
$$

(16)

where the coordinate of the light quark is on the light cone i.e., $z^2 = 0$ and $z_+ = 0$. $n_+^\mu = (1, 0, 0)$ and $n_-^\mu = (0, 1, 0)$ are the light cone vectors. $f_B$ is the decay constant. $\phi_B^+$ and $\phi_B^-$ are respectively the leading- and sub-leading-twist WFs. The properties and relations of $\phi_B^\pm$ are listed as follows.

$$
\int_0^1 dx \phi_{B1}^+(x) = 1,
$$

(17)

$$
\phi_{B1} = \phi_B^+,
$$

(18)

$$
\phi_{B2} = \phi_B^+ - \phi_B^-,
$$

(19)

$$
\phi_B^+(x) + x \phi_B^-(x) = 0,
$$

(20)

where $x$ is the longitudinal momentum fraction carried by the light quark in the $B$ meson. $\phi_B^+$ and $\phi_B^-$ have different asymptotic behaviors as $x \to 0$, $\phi_B^+ \sim x$ but $\phi_B^-$ will not vanish. So they do not coincide, i.e., $\phi_B^+ \neq \phi_B^- \neq 0$. In many actual calculations of nonleptonic
$B$ decays, only the contributions of $\phi_{B1}$ are considered appropriately, while those of $\phi_{B2}$ are assumed to be power suppressed and almost completely neglected. However, studies of Refs. [30–34] have shown that contributions of $\phi_{B2}$ to the $B \to \pi$ transition formfactors with the pQCD approach could have a large proportion rather than negligible. For example, the share could reach up to $\sim 30\%$ for some specific cases [30, 31]. Clearly, the contributions of $\phi_{B2}$ will have some impacts on branching ratios of $B$ meson decays. We should pay due attention to contributions of $\phi_{B2}$ in pace with the improvements of measurement precision, which is one main motivation of this work. The contributions of $\phi_{B2}$ to the $B \to PP$ decays have been studied with the QCDF approach [35]. The study of Ref. [35] showed that $\phi_{B2}$ only contributed to nonfactorizable annihilation amplitudes, and is helpful in explaining pure annihilation $B$ decays. Different from the QCDF case, $\phi_{B2}$ will contribute to both factorizable and nonfactorizable emission amplitudes with the pQCD approach, besides the nonfactorizable annihilation amplitudes. That is to say, $\phi_{B2}$ would have much more influence on nonleptonic $B$ decays with the pQCD approach when compared with the QCDF approach. However, the contributions of $\phi_{B2}$ to the $B \to PP$ decays have not been studied with the pQCD approach, which is the focus of this paper.

One candidate of the most often used leading $B$ mesonic WF $\phi^+_B$ in earlier studies with the pQCD approach is written as [25]

$$
\phi^+_B(x, b) = N x^2 \bar{x}^2 \exp \left\{ - \left( \frac{m_B x}{\sqrt{2} \omega_B} \right)^2 - \frac{1}{2} \omega_B^2 b^2 \right\}, \tag{21}
$$

where $b$ is the conjugate variable of the transverse momentum $k_T$. $\bar{x} = 1 - x$. $\omega_B$ is the shape parameter. $N$ is the normalization constant.

$$
\int_0^1 dx \phi^+_B(x, 0) = 1. \tag{22}
$$

The corresponding sub-leading $B$ mesonic WF $\phi^-_B$ [31] can be obtained by solving the equation of motion given by Eq.(20).

$$
\phi^-_B(x, b) = N \frac{2 \omega_B^4}{m_B^4} \exp \left( - \frac{1}{2} \omega_B^2 b^2 \right) \left\{ \sqrt{\pi} \frac{m_B}{\sqrt{2} \omega_B} \operatorname{Erf} \left( \frac{m_B}{\sqrt{2} \omega_B}, \frac{x m_B}{\sqrt{2} \omega_B} \right) + \left[ 1 + \left( \frac{m_B \bar{x}}{\sqrt{2} \omega_B} \right)^2 \right] \exp \left( - \left( \frac{x m_B}{\sqrt{2} \omega_B} \right)^2 \right) \right\}. \tag{23}
$$

In addition, according to the convention of Refs. [36, 37], WFs of the final pseudoscalars $\pi^+$ and $K^+$ are generally written as follows.

$$
\langle M(p) | \bar{q}_\alpha(0) u_\beta(z) | 0 \rangle
$$
\[ \phi_M^a(x) = 6x \bar{x} \left\{ 1 + a_1^M C^{3/2}_1(\xi) + a_2^M C^{3/2}_2(\xi) \right\}, \]

\[ \phi_M^p(x) = 1 + 3 \rho_+^M - 9 \rho_-^M a_1^M + 18 \rho_+^M a_2^M \\
+ \frac{3}{2} (\rho_+^M + \rho_-^M) (1 - 3a_1^M + 6a_2^M) \ln(x) \\
+ \frac{3}{2} (\rho_+^M - \rho_-^M) (1 + 3a_1^M + 6a_2^M) \ln(\bar{x}) \\
- \frac{3}{2} \rho_-^M - \frac{27}{2} \rho_+^M a_1^M + 27 \rho_-^M a_2^M ) C^{1/2}_1(\xi) \\
+ (30 \eta_M - 3 \rho_-^M a_1^M + 15 \rho_+^M a_2^M ) C^{1/2}_2(\xi), \]

\[ \phi_M^t(x) = \frac{3}{2} (\rho_-^M - 3 \rho_+^M a_1^M + 6 \rho_-^M a_2^M) \\
- C^{1/2}_1(\xi) \left\{ 1 + 3 \rho_+^M - 12 \rho_-^M a_1^M + 24 \rho_+^M a_2^M \\
+ \frac{3}{2} (\rho_+^M + \rho_-^M) (1 - 3a_1^M + 6a_2^M) \ln(x) \\
+ \frac{3}{2} (\rho_+^M - \rho_-^M) (1 + 3a_1^M + 6a_2^M) \ln(\bar{x}) \right\} \\
- 3 (3 \rho_+^M a_1^M - 15 \rho_-^M a_2^M ) C^{1/2}_2(\xi), \]

where the variable \( \xi = x - \bar{x} = 2x - 1 \). The normalization conditions are

\[ \int_0^1 dx \phi_M^a(x) = 1, \]

\[ \int_0^1 dx \phi_M^p(x) = 0. \]

Other parameters are expressed as \[37\]: \( \rho_+^M = \frac{m_K^2}{\mu_3^M}, \rho_-^K \simeq \frac{m_8}{\mu_K}, \rho_-^\pi = 0, \) and \( \eta_M = \frac{f_{3M}}{f_M \mu_M}. \)

The Gegenbauer polynomials are written as follows.

\[ C^{1/2}_1(\xi) = \xi, \]

\[ C^{3/2}_1(\xi) = 3 \xi, \]

\[ C^{1/2}_2(\xi) = \frac{3}{2} \xi^2 - \frac{1}{2}, \]
\[ C_{3/2}^{B}(\xi) = \frac{15}{2} \xi^2 - \frac{3}{2}. \] (33)

The curves of the normalized DAs \( \phi_{B}^{\pm}(x,0) \) and \( \phi_{B}^{-}(x,0) \) for \( B \) meson in Eq.(21) and Eq.(23) are displayed in Fig.1. It can be clearly seen from Fig.1 that (1) DAs \( \phi_{B}^{\pm} \) are very asymmetric, and peak at small \( x \) region. This fact is generally consistent with the plausible suspicion that the light quark shares a small momentum fraction in \( B \) meson. In addition, DAs \( \phi_{B}^{+} \) vanish as \( x \rightarrow 1 \), and thus offer a natural cutoff on the seemingly counterintuitive contributions from large \( x \) domain. (2) \( \phi_{B}^{-} \) and \( \phi_{B2} \) do not vanish as \( x \rightarrow 0 \), thus the integral \( \int dx \frac{\phi_{B2}}{x} \) and \( \int dx \frac{\phi_{B2}}{x^2} \) corresponding to the factorizable emission topologies (form factors) diverge at the endpoint \( x = 0 \), as discussed in Ref. [29] with the collinear approximation. This implies that, on the one hand, the contributions of \( \phi_{B2} \) might be important at small \( x \) regions and should be given due consideration in calculation, although \( \phi_{B}^{-} \) is sub-leading twist; on the other hand, it seems reasonable and necessary to retain the contributions of the transverse momentum to regulate the singularities at the endpoint with the pQCD approach.

The line shapes of DAs \( \phi_{M}^{\alpha,p,t}(x) \) for \( \pi \) and \( K \) mesons in Eq.(25), Eq.(26) and Eq.(27) are shown in Fig. 2. The pionic DAs are totally symmetric with respect to the \( x \leftrightarrow \bar{x} \) exchange. The \( SU(3) \) breaking effects on kaonic DAs are considered. The quark-mass corrections modify the asymptotic behaviors of \( \phi_{M}^{p,t} \) and induce the logarithmic endpoint singularities, as analyzed in Ref. [37].

With the above mesonic DAs, we can obtain the hadron transition formfactors and amplitudes of the \( B \rightarrow PP \) decays with the pQCD approach. There are some conventions in our
FIG. 2: The shape lines of DAs $\phi_M^{a,p,t}$ for $K$ in (a) and $\pi$ in (b) versus $x$ (horizontal axis).

calculation. In the rest frame of $B$ meson, the light-cone kinematic variables of participating particles in the heavy quark limit are defined as follows.

$$p_B = p_1 = (p^+_1, p^-_1, \vec{p}_{1T}) = \frac{m_B}{\sqrt{2}}(1, 1, 0), \quad (34)$$

$$p_M = p_2 = (p^+_2, p^-_2, \vec{p}_{2T}) = \frac{m_B}{\sqrt{2}}(0, 1, 0), \quad (35)$$

$$p_M' = p_3 = (p^+_3, p^-_3, \vec{p}_{3T}) = \frac{m_B}{\sqrt{2}}(1, 0, 0), \quad (36)$$

$$k_1 = (x_1 p^+_1, 0, \vec{k}_{1T}), \quad (37)$$

$$k_2 = (0, x_2 p^-_2, \vec{k}_{2T}), \quad (38)$$

$$k_3 = (x_3 p^+_3, 0, \vec{k}_{3T}), \quad (39)$$

where $k_1$ and $x_1$ are respectively the momentum and longitudinal momentum fraction of light quark in the $B$ meson; $k_{2,3}$ and $x_{2,3}$ are respectively the momentum and longitudinal momentum fraction of anti-quark in final hadrons. $\vec{k}_{iT}$ is the transverse momentum. It is clear that $p_1^2 = m_B^2, p_2^2 = m_M^2 = 0$ and $p_3^2 = m_M'^2 = 0$.

The formfactors for the $B \to P$ transition are defined as [38]

$$\langle M(p_2) | (\bar{q} b)_{V-A} | B(p_1) \rangle = \left\{ (p_1 + p_2)^\mu - \frac{m_B^2 - m_M^2}{q^2} q^\mu \right\} F_1(q^2) + \frac{m_B^2 - m_M^2}{q^2} q^\mu F_0(q^2), \quad (40)$$
TABLE I: The values of the input parameters, where their central values will be regarded as the default inputs unless otherwise specified. The numbers in parentheses are errors.

| CKM parameters [1] | A = 0.790(17), | λ = 0.22650(48), |
|-------------------|----------------|-----------------|
|                   | ρ = 0.141(17), | η = 0.357(11),  |
| mass of the particles [1] | m_{π^0} = 134.98 MeV, | m_{π^±} = 139.57 MeV, |
|                   | m_{K^0} = 497.61 MeV, | m_{K^±} = 493.68 MeV, |
|                   | m_{B_u} = 5279.34(12) MeV, | m_{B_d} = 5279.65(12) MeV, |
|                   | m_b = 4.78(6) GeV, | m_s = 130.0(1.8) MeV [39], |
| decay constants [1] | f_π = 130.2(1.2) MeV, | f_{3π} = 0.45(15) × 10^{-2} GeV^2 [37], |
|                   | f_K = 155.7(3) MeV, | f_{3K} = 0.45(15) × 10^{-2} GeV^2 [37], |
|                   | f_B = 190.0(1.3) MeV, |
| lifetime [1]       | τ_{B^±} = 1.638(4) ps, | τ_{B^±} = 1.519(4) ps, |
| Gegenbauer moments at the scale of μ = 1 GeV [37] | a_{π}^1 = 0, | a_{π}^2 = 0.25(15), |
|                   | a_{K}^1 = 0.06(3), | a_{K}^2 = 0.25(15). |

FIG. 3: Feynman diagrams contributing to the $\overline{B} \to M$ formfactors, where the dots denote appropriate current interactions, and boxes denote quark scattering amplitudes.

where $q = p_1 - p_2$. It is required that $F_0(0) = F_1(0)$ at the pole of $q^2 = 0$.

The lowest order Feynman diagrams for the $B \to M$ transition formfactors are shown in Fig.3. The formfactors $F_i$ are written as the convolution integrals of the quark scattering amplitudes $\mathcal{T}$ and hadron WFs $\Phi_i$ with the pQCD approach.

$$F_i = \int dx_1 dx_2 db_1 db_2 \Phi_B(x_1, b_1) e^{-s_B} \mathcal{T}(x_1, x_2, b_1, b_2) \Phi_M(x_2, b_2) e^{-s_M},$$

where $b_i$ is the conjugate variable of transverse momentum $k_{iT}$. The Sudakov factors $e^{-s_B}$ and $e^{-s_M}$ are introduced for WFs $\Phi_B$ and $\Phi_M$, respectively. The Sudakov factor is a char-
acteristic element and highly recommended by the pQCD approach to effectively regulate the nonperturbative contributions, so that a dominant share of formfactor would come from hard gluon exchange, and the perturbative calculation would be reasonable and practicable. The expressions for formfactors including the $\phi_{B2}$ contributions are listed in Appendix A. Our results of formfactors are shown in Fig. 4, 5, 6 and Table II.

![Contour plots](image)

FIG. 4: Contour plot of $F_0^{B \to \pi}(0)$. The values of formfactors denoted by shades. The values in (a,b) and (c,d) are calculated without and with the contributions from $\phi_{B2}$.

The dependences of formfactor $F_0^{B \to \pi}(0)$ on some input parameters are shown in Fig. 4. It is seen clearly that (1) formfactors obtained with the pQCD approach are sensitive to the shape parameter $\omega_B$ for $B$ mesonic WFs. This phenomenon is basically analogical with that of Ref. [31]. (2) the effects of the chiral mass $\mu_M$ indicate the importances of the twist-3 contributions. It is shown in Ref. [31] that the contributions from twist-3 $\phi_{\pi}^{p,t}$ to
FIG. 5: Formfactors of $F_{B \rightarrow \pi}^0(q^2)$ and $F_{B \rightarrow K}^0(q^2)$ versus $q^2$. The bands in (a,b) correspond to the contributions from WFs $\phi_{B1}$ and $\phi_{B2}$. The bands in (c,d) correspond to the contributions from Fig. 3 (a) and (b). The bands are calculated with $\omega_B = 0.41 \sim 0.45$ GeV and $\mu_M = 1.5 \sim 1.7$ GeV. The lines correspond the S2 scenario.

$F_{0}^{B \rightarrow \pi}(0)$ could exceed 50% with appropriate parameters. (3) The contributions of WF $\phi_{B2}$ can enhance the formfactors. By comparison of the branching ratios for $B \rightarrow PP$ decays with the experimental results, three optimal scenarios are obtained, when the $\phi_{B2}$ is considered.

Scenario 1 (S1) : $\omega_B = 0.45$ GeV and $\mu_M = 1.7$ GeV for PDG data;  
Scenario 2 (S2) : $\omega_B = 0.43$ GeV and $\mu_M = 1.6$ GeV for Belle data;  
Scenario 3 (S3) : $\omega_B = 0.41$ GeV and $\mu_M = 1.5$ GeV for BaBar data.

The formfactors are assumed to be perturbatively calculable with the pQCD approach, but reliable only for the large recoil transition, i.e., the small $q^2$ regions. Thus in this paper, the formfactors with $q^2 \leq 4$ GeV$^2$ are calculated. The dependences of formfactors $F_{0}^{B \rightarrow \pi}(q^2)$ and $F_{0}^{B \rightarrow K}(q^2)$ on $q^2$ and are shown in Fig. 5. It is seen clearly that (1) the formfactors $F_0$ increase monotonically and slowly with $q^2$ within the large recoil domains. (2) The lion’s
FIG. 6: The percentages of contributions to $F_0^{B\to\pi}(0)$ from different ranges of $\alpha_s/\pi$ for the S2 scenario. The numbers over histogram denote the total percentages. The histograms in (a) correspond to the contributions from WFs $\phi_B^1$ and $\phi_B^2$. The histograms in (b) correspond to the contributions from Fig.3 (a) and (b).

TABLE II: The numerical values of formfactors $F_0^{B\to\pi}$ and $F_0^{B\to K}$. The contributions from $\phi_B^1$, $\phi_B^2$, Fig.3 (a) and Fig.3 (b) are given in the corresponding rows. The uncertainties in parentheses arise from variations of $\omega_B \pm 0.01$ GeV, $\mu_M \pm 0.1$ GeV, and $a_2^M \pm 0.15$, respectively.

| transition | case | S1 | S2 | S3 |
|------------|------|----|----|----|
| $F_0^{B\to\pi}(0)$ | $\phi_B^1$ | 0.190(06)(08)(08) | 0.186(06)(07)(08) | 0.181(06)(07)(07) |
| | $\phi_B^2$ | 0.041(01)(00)(05) | 0.039(01)(00)(04) | 0.037(01)(00)(04) |
| | Fig. 3 (a) | 0.156(04)(03)(13) | 0.152(04)(03)(12) | 0.147(04)(03)(12) |
| | Fig. 3 (b) | 0.074(03)(05)(00) | 0.073(03)(04)(00) | 0.071(03)(04)(00) |
| | total | 0.231(07)(07)(13) | 0.224(07)(07)(12) | 0.218(06)(06)(12) |
| $F_0^{B\to K}(0)$ | $\phi_B^1$ | 0.235(08)(12)(09) | 0.231(07)(11)(09) | 0.227(07)(10)(09) |
| | $\phi_B^2$ | 0.051(01)(00)(05) | 0.049(01)(00)(05) | 0.047(01)(00)(05) |
| | Fig. 3 (a) | 0.193(05)(06)(13) | 0.189(05)(05)(14) | 0.185(04)(05)(13) |
| | Fig. 3 (b) | 0.093(04)(06)(00) | 0.091(04)(05)(01) | 0.089(04)(05)(01) |
| | total | 0.286(09)(12)(14) | 0.280(08)(11)(14) | 0.274(08)(10)(14) |

The share of formfactors is from B mesonic WFs $\phi_B^1$, and the share of $\phi_B^2$ is relatively small. This is why the contributions from B mesonic WFs $\phi_B^2$ were usually not considered in most of previous works. Our results in Table II show that the contributions from $\phi_B^2$ to formfactors $F_0^{B\to\pi}(0)$ and $F_0^{B\to K}(0)$ are about 17%, which is much larger than 7% from the
next-to-leading order (NLO) contributions \cite{40}. (3) More than half of the formfactors is from the contributions of topology Fig. 3 (a), about 67% shown in Table II.

In Fig. 6, more details about the contributions from \( \phi_{B1} \) and \( \phi_{B2} \), from topology Fig. 3 (a) and (b) to formfactor \( F_{0}^{B\to\pi}(0) \) at \( q^2 = 0 \) are displayed bin by bin with respect to the distributions of \( \frac{\alpha_s}{\pi} \). It shows that about 90% of formfactor comes from the region of \( \frac{\alpha_s}{\pi} \leq 0.2 \), where the contributions from \( \phi_{B1} \) and \( \phi_{B2} \) account for more than 70% and 15%, the contributions from Fig. 3 (a) and (b) account for more than 55% and 30%, respectively. These results may imply that the quark scattering amplitudes are dominated by hard gluon exchange, and the perturbative calculation of the formfactor with the pQCD approach is feasible and reliable. An important and possible underlying mechanism is the way of choosing the hard scale as the maximum virtuality of quarks and gluons, see Eq.(A15), besides the suppression of the long-distance contributions from Sudakov factors.

The values of formfactors in Table II are less than those of Refs. \[30,31\], due to different DAs models and different values of input parameters. As is shown in Fig. 4, the formfactors decrease with the increase of shape parameter \( \omega_{B} \). A large shape parameter \( \omega_{B} \) for B mesonic WFs is used in our calculation, compared with that in Ref. \[31\]. It should be pointed out that a relatively small value of formfactor \( F_{0}^{B\to\pi}(0) \) has recently been obtained by fitting the Bourrely-Lellouch-Caprini parametrization \[41\] with the available experimental data and theoretical informations and then extrapolating to the point of \( q^2 = 0 \), for example, 0.254\(^{+0.033}_{-0.022}\) in Ref. \[41\], 0.248\(\pm0.082\) in Ref. \[42\], 0.20\(\pm0.14\) in Ref. \[43\], 0.254\(\pm0.081\) in Ref. \[44\]. Our results of \( F_{0}^{B\to\pi}(0) \) are basically consistent those of Refs. \[41–44\] within uncertainties. In addition, from the definition of formfactor in Eq.(40), it is clear that there should be a relation between formfactors and decay constants,

\[
\frac{F_{0}^{B\to\pi}(0)}{F_{0}^{B\to K}(0)} \approx \frac{f_{\pi}}{f_{K}}.
\] (42)

The numbers in Table II hold this relation well. The small violation arises from the \( SU(3) \) flavor breaking effects.

The Feynman diagrams for two-body nonleptonic \( B \) meson decays are shown in Fig. 7. The amplitudes \( \mathcal{A} \) with the pQCD approach are usually divided into three parts: the short-distance contributions encoded in the Wilson coefficients \( C_{i} \), the quark scattering amplitudes

\[^{a}F_{0}^{B\to\pi}(0) = f_{\pi}(0) \text{ is assumed.}\]
The general form of decay amplitude is

$$A_i \propto \int \prod_j dx_j \, db_j \, C_i(t_i) \, T_i(t_i, x_j, b_j) \, \Phi_j(x_j, b_j) e^{-S_j}. \quad (43)$$

In the rest frame of the $B$ meson, the $CP$-averaged branching ratios are defined as:

$$Br = \frac{\tau_B}{16\pi \, m_B^2} \left\{ |A(B \to f)|^2 + |A(\bar{B} \to \bar{f})|^2 \right\}, \quad (44)$$

where $\tau_B$ is the lifetime of the $B$ meson. $p_{cm}$ is the common momentum of final states. The decay amplitudes including the $\phi_{B2}$ contributions are listed in Appendix B. For the charged $B_u$ meson decays, the $CP$ violating asymmetries arises from the interference between tree and penguin amplitudes. The direct $CP$ violating asymmetry is defined as follows.

$$A_{CP} = \frac{\Gamma(B^- \to f) - \Gamma(B^+ \to \bar{f})}{\Gamma(B^- \to f) + \Gamma(B^+ \to \bar{f})} = \frac{|A(B^- \to f)|^2 - |A(B^+ \to \bar{f})|^2}{|A(B^- \to f)|^2 + |A(B^+ \to f)|^2}. \quad (45)$$

For the neutral $B_d$ meson decays into final state $f$ with $f = \bar{f}$, the time-dependent $CP$ violating asymmetry is defined as follows.

$$A_{CP} = \frac{\Gamma(\bar{B}^0 \to \bar{f}) - \Gamma(B^0 \to f)}{\Gamma(\bar{B}^0 \to \bar{f}) + \Gamma(B^0 \to f)} \approx S_f \sin(x \, \Gamma \, t) - C_f \cos(x \, \Gamma \, t), \quad (46)$$
with the $y = \frac{\Delta \Gamma}{2 \Gamma_B} \simeq 0$ approximation, where $x = \frac{\Delta m_B}{\Gamma_B} = 0.769(4)$ [1] is the $B^0-\bar{B}^0$ oscillation parameter. $\Gamma_B = \frac{1}{\tau_B}$ is the full width of the $B_d$ meson. $C_f$ and $S_f$ are the direct and mixing-induced $CP$ asymmetries.

$$C_f = \frac{1 - |\lambda_f|^2}{1 + |\lambda_f|^2},$$

$$S_f = \frac{2 \Im m(\lambda_f)}{1 + |\lambda_f|^2},$$

$$\lambda_f = \frac{V_{tb}^* V_{td}}{V_{tb} V_{td}^*} \mathcal{A}(\bar{B}^0 \to f).$$

**TABLE III:** The $CP$-averaged branching ratios $Br$ (in the unit of $10^{-6}$) for the $B_u \to PP$ decays.

The theoretical results are respectively calculated with parameters of S1, S2, S3 scenarios to compare with data of PDG, Belle and BaBar [1]. The theoretical uncertainties arise from variations of $\omega_B \pm 0.01$ GeV, $\mu_M \pm 0.1$ GeV, and $\phi_2^M \pm 0.15$, respectively.

| mode      | $B^- \to \pi^-\pi^0$ | $B^- \to \pi^-\bar{K}^0$ | $B^- \to \pi^0K^-$ | $B^- \to K^0K^-$ |
|-----------|----------------------|--------------------------|-------------------|------------------|
| PDG       | 5.5 ± 0.4            | 23.7 ± 0.8               | 12.9 ± 0.5        | 1.31 ± 0.17      |
| S1 $\phi_{B1}+\phi_{B2}$ | 3.04 ± 0.18 + 0.19 ± 0.27 | 24.12 ± 1.73 + 3.69 ± 2.50 | 13.13 ± 0.93 + 1.95 ± 1.11 | 1.95 ± 0.13 + 0.34 ± 0.18 |
| $\phi_{B1}$ | 2.16 ± 0.14 + 0.15 ± 0.15 | 17.89 ± 1.36 + 2.97 ± 1.30 | 9.71 ± 0.73 + 1.57 + 0.58 | 1.45 + 0.11 + 0.27 + 0.07 |
| S2 $\phi_{B1}+\phi_{B2}$ | 3.23 ± 0.19 + 0.18 ± 0.29 | 23.87 ± 1.72 + 3.83 ± 2.51 | 13.03 ± 0.93 + 2.03 + 1.12 | 1.88 ± 0.13 + 0.35 + 0.17 |
| $\phi_{B1}$ | 2.27 ± 0.15 + 0.17 ± 0.15 | 17.64 ± 1.36 + 3.08 ± 1.30 | 9.60 ± 0.74 + 1.64 ± 0.59 | 1.38 ± 0.10 ± 0.29 + 0.06 |
| Belle     | 5.86 ± 0.46          | 23.97 ± 0.89             | 12.62 ± 0.64      | 1.11 ± 0.20      |
| S3 $\phi_{B1}+\phi_{B2}$ | 3.42 ± 0.21 + 0.20 ± 0.32 | 23.49 ± 1.71 + 3.96 ± 2.51 | 12.87 ± 0.93 + 2.11 + 1.12 | 1.79 ± 0.12 + 0.36 + 0.15 |
| $\phi_{B1}$ | 2.39 ± 0.16 + 0.18 ± 0.16 | 17.30 ± 1.35 + 3.19 ± 1.30 | 9.44 ± 0.73 + 1.70 ± 0.59 | 1.30 ± 0.10 + 0.29 + 0.05 |
| BaBar     | 5.02 ± 0.54          | 23.9 ± 1.5               | 13.6 ± 0.9        | 1.61 ± 0.45      |

The numerical results on the $CP$-averaged branching ratios together with experimental data are presented in Table III and IV, $CP$ asymmetries in Table V and VI. Using the minimum $\chi^2$ method,

$$\chi^2 = \sum_i \frac{(B_{i,\text{theo.}} - B_{i,\text{exp.}})^2}{\sigma^2_{B_{i,\text{exp.}}}},$$

three optimal scenarios (S1, S2 and S3) of parameters $\omega_B$ and $\mu_M$ are obtained when the contributions of $\phi_{B2}$ are considered. For the ten concerned $B$ decay modes, $\chi^2/d.o.f =$
TABLE IV: The numerical values of the $CP$-averaged branching ratios (in the unit of $10^{-6}$) for the $B_d \to PP$ decays. Other legends are the same as those of Table. III.

| mode | $\mathcal{B}^0 \to \pi^+\pi^-$ | $\mathcal{B}^0 \to \pi^0\pi^0$ | $\mathcal{B}^0 \to \pi^+K^-$ |
|------|-------------------------------|-------------------------------|-------------------------------|
| PDG  | $5.12\pm0.19$                | $1.59\pm0.26$                | $19.6\pm0.5$                |
| S1   | $\phi_{B1}\phi_{B2}$         | $\phi_{B1}$                   | $\phi_{B1}$                   |
|      | $5.52\pm0.34+0.37\pm0.47$    | $3.81\pm0.25\pm0.31\pm0.23$  | $20.07\pm1.44+3.13\pm2.05$  |
|      | $-0.32\pm0.36\pm0.43$        | $-0.23\pm0.30\pm0.20$        | $-0.02\pm0.03\pm0.01$       |
|      | $0.24\pm0.02\pm0.04\pm0.01$  | $0.19\pm0.01\pm0.03\pm0.02$  | $15.00\pm1.14+2.53\pm1.07$  |
|      | $-0.02\pm0.03\pm0.01$        | $-0.01\pm0.03\pm0.01$        | $-1.05\pm2.25\pm1.02$       |
| Belle| $5.04\pm0.28$                | $1.31\pm0.27$                | $20.00\pm0.69$                |
| S2   | $\phi_{B1}\phi_{B2}$         | $\phi_{B1}$                   | $\phi_{B1}$                   |
|      | $5.82\pm0.36+0.41\pm0.46$    | $3.99\pm0.26+0.34\pm0.24$    | $19.81\pm1.43+3.24\pm2.05$  |
|      | $-0.34\pm0.39\pm0.46$        | $-0.25\pm0.33\pm0.21$        | $-0.02\pm0.04\pm0.01$       |
|      | $0.24\pm0.02\pm0.04\pm0.01$  | $0.18\pm0.01\pm0.03\pm0.02$  | $14.76\pm1.14+2.62\pm1.07$  |
|      | $-0.02\pm0.04\pm0.01$        | $-0.01\pm0.03\pm0.01$        | $-1.05\pm2.32\pm1.02$       |
| BaBar| $5.5\pm0.5$                  | $1.83\pm0.25$                | $19.1\pm0.8$                 |
| S3   | $\phi_{B1}\phi_{B2}$         | $\phi_{B1}$                   | $\phi_{B1}$                   |
|      | $6.12\pm0.39+0.45\pm0.54$    | $4.16\pm0.28+0.37\pm0.26$    | $19.45\pm1.42+3.34\pm2.04$  |
|      | $-0.36\pm0.43\pm0.50$        | $-0.26\pm0.36\pm0.23$        | $-0.02\pm0.04\pm0.01$       |
|      | $0.23\pm0.02\pm0.04\pm0.01$  | $0.18\pm0.01\pm0.03\pm0.02$  | $14.43\pm1.13+2.70\pm1.06$  |
|      | $-0.02\pm0.04\pm0.01$        | $-0.01\pm0.03\pm0.01$        | $-1.04\pm2.38\pm1.01$       |

92.9/8, 73.1/8 and 56.4/7 correspond to data of PDG, Belle and BaBar, respectively. The agreement between theoretical and experimental results is illustrated by the $\chi^2$ distribution in Fig. 8. The followings are our comments.

(1) From Table III and IV, it is seen that the contributions of WF $\phi_{B2}$ are more than 25% of total branching ratios, except for the pure annihilation $\mathcal{B}^0 \to K^+K^-$ decay. That is because WF $\phi_{B2}$ contributes nothing to the factorizable annihilation amplitudes of Eqs.(C13)-(C18). From Table V and VI, it is seen that the contributions of WF $\phi_{B2}$ result in a small
proportional to the CKM factor.

TABLE V: The $CP$ asymmetries $A_{CP}$ (in the unit of $10^{-2}$) for $B \to PP$ decays. Other legends are the same as those of Table III.

| $A_{CP}$ | $\pi^-\pi^0$ | $\pi^-\bar{K}^0$ | $\pi^0K^-$ | $K^0\bar{K}^-$ | $\pi^+\bar{K}^-$ |
|----------|---------------|-------------------|-------------|----------------|-----------------|
| PDG      | 3±4           | -1.7±1.6          | 3.7±2.1     | 4±14           | -8.3±0.4        |
| $\phi_{B_1}+\phi_{B_2}$ | -0.004        | -0.67±0.02±0.04±0.14 | -6.25±0.25±0.30±1.51 | 14.78±0.27±1.05±3.33 | -7.39±0.29±0.41±1.98 |
| $\phi_{B_1}$ | -0.02         | -0.74±0.02±0.04±0.14 | -6.74±0.30±0.36±1.74 | 14.83±0.26±1.10±3.28 | -8.14±0.33±0.49±2.38 |
| Belle    | 2.5±4.4       | -1.1±2.2          | 4.3±2.4     | 1.4±16.8       | -6.9±1.6        |
| $\phi_{B_1}+\phi_{B_2}$ | -0.01         | -0.69±0.02±0.05±0.15 | -6.09±0.25±0.30±1.43 | 15.28±0.28±1.21±3.53 | -7.98±0.28±0.41±1.91 |
| $\phi_{B_1}$ | -0.02         | -0.75±0.02±0.05±0.15 | -6.51±0.29±0.36±1.66 | 15.39±0.27±1.30±3.55 | -7.98±0.33±0.50±2.31 |
| BaBar    | 3±8           | -2.9±4.0          | 3±4         | 10±26          | -10.7±1.7       |
| $\phi_{B_1}+\phi_{B_2}$ | -0.01         | -0.70±0.02±0.05±0.16 | -5.86±0.24±0.30±1.36 | 15.90±0.29±1.41±3.78 | -7.03±0.28±0.41±1.84 |
| $\phi_{B_1}$ | -0.03         | -0.77±0.02±0.05±0.16 | -6.30±0.29±0.36±1.57 | 16.12±0.29±1.56±3.89 | -7.89±0.33±0.50±2.24 |

FIG. 8: The $\chi^2$ distribution of branching ratios.

reduction of direct $CP$ asymmetries.

(2) From appendix B, it is clearly seen that for the $B \to \pi\pi$ and $KK$ decays, the CKM factors of the tree and penguin amplitudes are respectively $V_{ub}V_{ud}^*$ and $V_{tb}V_{td}^*$, and have the same order of magnitude $\propto \lambda^3$. For the $B \to \pi K$ decays, the tree amplitudes being proportional to the CKM factor $V_{ub}V_{us}^*$ are suppressed by $\lambda^2$ compared with the penguin
the decays, as analyzed in Ref. \[\phi\] that penguin contributions are dynamically enhanced and essentially for explaining $B\to\pi^{0}\pi^{0}$ amplitudes being proportional to the CKM factor $V_{tb}V_{ts}^{\ast}$. In addition, the theoretical and experimental results in Table III and IV show that branching ratios for $B\to\pi K$ decays are indeed greater than those for $B\to\pi\pi$ and $\overline{K}K$ decays. These facts confirm previous studies [6, 10] that penguin contributions are dynamically enhanced and essential for explaining the $B\to\pi K$ decays. What’s more, our studies show that the nonfactorizable annihilation amplitudes mainly from WF $\phi_{B1}$ rather than $\phi_{B2}$ provide large strong phases for the $B\to\pi K$ decays, as analyzed in Ref. [10].

### Table VI: The $CP$ Asymmetries (in the unit of $10^{-2}$) for $B_{d}\to PP$ Decays

|        | $C_{\pi^{+}\pi^{-}}$ | $S_{\pi^{+}\pi^{-}}$ | $C_{\pi^{0}\pi^{0}}$ | $S_{\pi^{0}\pi^{0}}$ |
|--------|----------------------|----------------------|----------------------|----------------------|
| PDG    | −32±4                | −65±4                | −33±22               |                      |
| $\phi_{B1}+\phi_{B2}$ | −17.85±0.55+0.05+3.84 | −81.91±0.17+1.57+2.43 | 38.34±1.30+1.78+5.37 | 89.03±0.49+1.13+0.97 |
| $\phi_{B1}$   | −21.52±0.71+0.13+4.96 | −86.19±0.15+1.65+2.94 | 39.06±1.60+1.86+4.49 | 85.90±0.53+1.32+0.35 |
| Belle       | −33±7                | −64±9                | −14±37               |                      |
| $\phi_{B1}+\phi_{B2}$ | −16.75±0.51+0.05+3.32 | −83.12±0.16+1.55+2.34 | 37.29±1.41+1.91+5.29 | 88.69±0.50+1.31+0.83 |
| $\phi_{B1}$ | −20.24±0.66+0.12+4.57 | −81.46±0.15+1.64+2.86 | 37.65±1.63+2.01+4.49 | 85.41±0.54+1.54+0.34 |
| BaBar       | −25±8                | −68±10               | −43±26               |                      |
| $\phi_{B1}+\phi_{B2}$ | −15.72±0.48+0.05+3.23 | −84.33±0.15+1.53+2.24 | 36.32±1.43+2.08+5.21 | 88.11±0.50+1.55+0.70 |
| $\phi_{B1}$ | −19.04±0.63+0.12+4.20 | −82.79±0.14+1.62+2.77 | 36.33±1.66+2.22+4.47 | 84.65±0.55+1.83+0.37 |

|        | $C_{\pi^{0}\kappa^{0}}$ | $S_{\pi^{0}\kappa^{0}}$ | $C_{K^{+}\kappa^{-}}$ | $S_{K^{+}\kappa^{-}}$ |
|--------|--------------------------|--------------------------|----------------------|----------------------|
| PDG    | 0±13                     | 58±17                    |                     |                      |
| $\phi_{B1}+\phi_{B2}$ | −0.54±0.01+0.05+0.25 | 68.74±0.02+0.16+0.20 | −81.17±0.45+0.79+0.13 | −28.21±0.94+1.59+0.95 |
| $\phi_{B1}$ | −0.85±0.01+0.06+0.36 | 69.29±0.03+0.18+0.13 | −82.90±0.46+0.67+0.27 | −28.35±1.02+1.25+0.35 |
| Belle  | −14±14                   | 67±32                    |                     |                      |
| $\phi_{B1}+\phi_{B2}$ | −0.60±0.01+0.05+0.27 | 68.86±0.02+0.18+0.20 | −81.26±0.44+0.88+0.11 | −27.97+0.94+1.66+0.24 |
| $\phi_{B1}$ | −0.93±0.01+0.07+0.39 | 69.40+0.04+0.21+0.15 | −83.11+0.44+0.76+0.25 | −27.65+1.01+1.35+0.75 |
| BaBar  | 13±13                    | 55±20                    |                     |                      |
| $\phi_{B1}+\phi_{B2}$ | −0.67±0.00+0.06+0.30 | 68.99±0.02+0.21+0.20 | −81.24+0.42+0.97+0.08 | −27.80+0.93+1.71+0.35 |
| $\phi_{B1}$ | −1.02±0.01+0.08+0.43 | 69.53±0.04+0.24+0.16 | −83.19+0.41+0.86+0.25 | −27.06+1.00+1.45+1.18 |
(3) From Fig. 8, it is seen that (i) for the $B \to \pi K$ decays, when the contributions of WF $\phi_{B_2}$ are included, theoretical results of branching ratio can give a satisfactory explanation on experimental data. Compared the numbers in Table III and IV with the NLO results of Refs. [11, 12, 45] (see Table VII), it is seen that the contributions of $\phi_{B_2}$ to branching ratios at the leading order (LO) is roughly equivalent to the NLO corrections without the participation of $\phi_{B_2}$. (ii) The consideration of WF $\phi_{B_2}$ cannot well settle the so-called $CP$ asymmetries “$K \pi$” puzzle, i.e. the discrepancy between theoretical and experimental results of $A_{CP}(B^- \to \pi^0 K^-) - A_{CP}(\bar{B}^0 \to \pi^+ K^-)$. The studies of Refs. [12, 45] showed that the NLO corrections including the glauber effects could flip the sign of $A_{CP}(B^- \to \pi^0 K^-)$. It should be noted that the NLO and NLOG theoretical uncertainties of branching ratios are still large, and the current measurement accuracy of $A_{CP}(B^- \to \pi^0 K^-)$ needs to be improved.

TABLE VII: The previous LO and NLO pQCD results for the $B \to \pi K$ decays, where NLO and NLOG denote without and with the glauber effects, the unit of branching ratios and direct $CP$ asymmetries are respectively $10^{-6}$ and $10^{-2}$.

| mode            | LO [11] | NLO [11] | NLOGb [12] | NLO [45] | NLOG [45] |
|-----------------|---------|----------|------------|----------|-----------|
| $Br(B^- \to \pi^- \bar{K}^0)$ | 17.0    | 24.5$^{+13.6}_{-8.1}$ | 21.1       | 27.2$^{+9.3}_{-6.7}$ | 24.1$^{+8.3}_{-6.0}$ |
| $Br(B^- \to \pi^0 K^-)$     | 10.2    | 13.9$^{+10.0}_{-5.6}$  | 12.9       | 15.3$^{+5.2}_{-3.8}$  | 14.0$^{+4.7}_{-3.5}$  |
| $Br(\bar{B}^0 \to \pi^+ K^-)$ | 14.2    | 20.9$^{+15.6}_{-8.3}$  | 17.7       | 23.3$^{+7.8}_{-5.7}$  | 21.7$^{+7.4}_{-5.3}$  |
| $Br(\bar{B}^0 \to \pi^0 \bar{K}^0)$ | 5.7     | 9.1$^{+5.6}_{-3.3}$   | 7.2        | 10.2$^{+3.4}_{-2.5}$  | 9.3$^{+3.2}_{-2.3}$   |
| $A_{CP}(B^- \to \pi^0 K^-)$  | $-8$    | $-1^{+3}_{-5}$         | $10$       | $-0.8^{+1.3}_{-1.4}$  | $2.1 \pm 1.6$         |
| $A_{CP}(\bar{B}^0 \to \pi^+ K^-)$ | $-12$   | $-9^{+6}_{-8}$         | $-11$      | $-7.6 \pm 1.7$       | $-8.1 \pm 1.7$        |

bThe glauber phases $S_c = S_{c1} = S_{c2} = -\frac{\pi}{2}$ is assumed.

(4) From Fig. 8 and Table III and IV, it is seen that for the $B \to \pi \pi$ decays, the pQCD results of branching ratios deviate from the current experimental measurement. The contributions of WF $\phi_{B_2}$ can enhance the branching ratios and reduce these deviations. Compared the numbers in Table III and IV with the NLO results of Refs. [11, 12, 46, 47] (see Table VIII), it is seen that (i) for the $\bar{B}^0 \to \pi \pi$ decays, the LO contributions of $\phi_{B_2}$ to branching ratios is roughly equivalent to the NLO corrections without the participation of $\phi_{B_2}$. (ii) Besides the large theoretical uncertainties, the pQCD results, including either WF
φ_{B_2} or the NLO contributions, cannot well explain data on branching ratio for the $\overline{B}^0 \rightarrow \pi^0 \pi^0$ decay and $CP$ asymmetries for the $\overline{B}^0 \rightarrow \pi^+ \pi^-$ decay.

TABLE VIII: The previous LO and NLO pQCD results for the $B \rightarrow \pi \pi$ decays. Other legends are the same as those of Table VII.

| mode                  | LO [11] | NLO [11] | NLOG\(^c\) [12] | LO [46] | NLO [46] | NLO [47] | NLOG [47] |
|-----------------------|---------|----------|-----------------|---------|----------|----------|----------|
| $Br(\overline{B}^- \rightarrow \pi^- \pi^0)$ | 3.5     | 4.0\(^{+3.4}_{-1.9}\) | 6.6             | 3.54    | 4.27\(^{+1.85}_{-1.47}\) | 3.35\(^{+1.10}_{-0.80}\) | 4.45\(^{+1.43}_{-1.06}\) |
| $Br(\overline{B}^0 \rightarrow \pi^+ \pi^-)$ | 7.0     | 6.5\(^{+6.7}_{-3.8}\) | 6.4             | 7.46    | 7.67\(^{+3.47}_{-2.64}\) | 6.19\(^{+2.12}_{-1.52}\) | 5.39\(^{+1.88}_{-1.33}\) |
| $Br(\overline{B}^0 \rightarrow \pi^0 \pi^0)$ | 0.12    | 0.29\(^{+0.50}_{-0.20}\) | 1.2             | 0.12    | 0.23\(^{+0.19}_{-0.15}\) | 0.29\(^{+0.11}_{-0.07}\) | 0.61\(^{+0.21}_{-0.17}\) |
| $C_f(\overline{B}^0 \rightarrow \pi^+ \pi^-)$ | -14     | -18\(^{+20}_{-12}\) | -17             | -27     | -12\(^{+4}_{-6}\) |
| $S_f(\overline{B}^0 \rightarrow \pi^+ \pi^-)$ | -34     | -43\(^{+100}_{-56}\) | -43             | -28     | -40\(^{+5}_{-4}\) |

\(^c\)The glauber phases $S_e = S_{e1} = S_{e2} = -\frac{\pi}{2}$ is assumed.

(5) For the $\overline{B}^0 \rightarrow \overline{K}K$ decays, the pQCD results with the contributions of WF $\phi_{B_2}$ are in good agreement with data of Belle and BaBar within uncertainties. But there are signs of tension between the pQCD results with the contributions of WF $\phi_{B_2}$ and experimental data for the $B^- \rightarrow K^0 K^-$ decay. In addition, from Table VI, there is a particularly interesting phenomenon that the direct $CP$ asymmetries $C_f$ is in general larger than the mixing-induced $CP$ asymmetries $S_f$ for the $B \rightarrow PP$ decays, but the opposite is true for the pure annihilation $\overline{B}^0 \rightarrow K^+ K^-$ decay.

In summary, the $B$ mesonic WF $\phi_{B_2}$ can contribute to emission amplitudes and nonfactorizable annihilation amplitudes with the pQCD approach. The enhancements from $\phi_{B_2}$ to hadronic transition formfactors and branching ratios for the nonleptonic $B \rightarrow PP$ decays are comparable with those from the NLO corrections without taking the $\phi_{B_2}$ into account. By considering $\phi_{B_2}$, the $B \rightarrow K \pi$ decays could be well explained at the LO levels. However, the LO contributions from $\phi_{B_2}$ cannot simultaneously settle the branching ratios and $CP$ asymmetries for the $\overline{B}^0 \rightarrow \pi \pi$ decays. A more careful study of the NLO corrections and other effects should be considered in the future. In addition, the contributions from $\phi_{B_2}$ result in a small reductions on the $CP$ asymmetries. All in all, the oft-ignored $\phi_{B_2}$ in previous studies should be given due attention in order to match the improvement of theoretical and experimental results.
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Appendix A: The formfactors for $B \rightarrow P$ transitions

Besides the definition of Eq.(40), another definition of formfactors is

$$\langle M(p_2) | (\bar{q} b)_{\nu A} | B(p_1) \rangle = p_1^\mu \tilde{f}_1 + p_2^\mu \tilde{f}_2 = (p_1 + p_2)^\mu f_+ + q^\mu f_-.$$  \hspace{1cm} (A1)

The relations among formfactors are

$$F_1 = f_+ = \frac{1}{2} (\tilde{f}_1 + \tilde{f}_2),$$  \hspace{1cm} (A2)

$$F_0 = \frac{1}{2} \tilde{f}_1 \left( 1 + \frac{q^2}{m_B^2} \right) + \frac{1}{2} \tilde{f}_2 \left( 1 - \frac{q^2}{m_B^2} \right).$$  \hspace{1cm} (A3)

Using the pQCDF formula of Eq.(41), the formfactors can be written as follows.

$$\tilde{f}_i = 2 \pi \frac{C_F}{N_c} m_B^2 f_M \left( \tilde{f}_i^a + \tilde{f}_i^b \right),$$  \hspace{1cm} (A4)

$$\tilde{f}_1^a = \int_0^1 dx_1 \int_0^1 dx_2 \int_0^\infty db_1 \int_0^\infty db_2 \alpha_s(t_a) S_t(x_2) H_{ab}(\alpha_g, \beta_a, b_1, b_2) e^{-S_B} e^{-S_M} \left[ \phi_{B1}(x_1, b_1) - \phi_{B2}(x_1, b_1) \right] \left[ \phi_M^a(x_2) - \phi_M^t(x_2) \right],$$  \hspace{1cm} (A5)

$$\tilde{f}_2^a = \int_0^1 dx_1 \int_0^1 dx_2 \int_0^\infty db_1 \int_0^\infty db_2 \alpha_s(t_a) S_t(x_2) H_{ab}(\alpha_g, \beta_a, b_1, b_2) e^{-S_B} e^{-S_M} \left\{ \phi_{B1}(x_1, b_1) \left[ \phi_M^a(x_2) \left( 1 + x_2 \eta \right) - 2 r_M x_2 \phi_M^p(x_2) \right] + 2 r_M \phi_M^t(x_2) \left( \frac{1}{\eta} - x_2 \right) - \phi_{B2}(x_1, b_1) \left[ r_M \phi_M^t(x_2) \left( \frac{1}{\eta} - x_2 \right) \right. \right. \right.$$  \hspace{1cm} \left. \left.$$

$$+ \phi_M^a(x_2) - r_M \phi_M^p(x_2) \left( \frac{1}{\eta} + x_2 \right) \right] \right\},$$  \hspace{1cm} (A6)

$$\tilde{f}_1^b = \int_0^1 dx_1 \int_0^1 dx_2 \int_0^\infty db_1 \int_0^\infty db_2 \alpha_s(t_b) S_t(x_1) H_{ab}(\alpha_g, \beta_b, b_2, b_1) e^{-S_B} e^{-S_M} x_1 \left\{ \phi_{B1}(x_1, b_1) \left[ \phi_M^a(x_2) \eta - 2 r_M \phi_M^p(x_2) \right] + \phi_{B2}(x_1, b_1) 2 r_M \phi_M^p(x_2) \right\},$$  \hspace{1cm} (A7)
\[ \tilde{f}_2^b = \int_0^1 dx_1 \int_0^1 dx_2 \int_0^\infty db_1 \int_0^\infty db_2 \alpha_s(t_b) S_t(x_1) H_{ab}(\alpha_g, \beta_g, b_2, b_1) \]

\[ e^{-S_B} e^{-S_M} \left\{ \phi_{B1}(x_1, b_1) \left[ 2 r_M \phi_M^p(x_2) \left( 1 + \frac{x_1}{\eta} \right) - x_1 \phi_M^a(x_2) \right] - \phi_{B2}(x_1, b_1) \phi_M^a(x_2) \frac{2 r_M x_1}{\eta} \right\}, \] (A8)

where \( N_c = 3 \) is the color number. The color factor \( C_F = \frac{N_c^2 - 1}{2 N_c} = 4 \). \( \alpha_s \) is the QCD coupling constant. \( r_M = \frac{\mu M}{m_B} \) and \( \eta = 1 - \frac{q^2}{m_B^2} \). The parameterization of \( S_t(x) \) can be found in Ref. [27]. Other parameters are written as follows.

\[ H_{ab}(\alpha, \beta, b_i, b_j) = b_i b_j K_0(b_i \sqrt{\alpha}) \left\{ \theta(b_i - b_j) K_0(b_j \sqrt{\beta}) I_0(b_j \sqrt{\beta}) + (b_i \leftrightarrow b_j) \right\}, \] (A9)

\[ S_B = s(x_1, b_1, p_1^+) + 2 \int_{1/b_1}^{t} \frac{d\mu}{\mu} \gamma_q, \] (A10)

\[ S_M = s(x_2, b_2, p_2^-) + s(\bar{x}_2, b_2, p_2^-) + 2 \int_{1/b_2}^{t} \frac{d\mu}{\mu} \gamma_q, \] (A11)

\[ \alpha_g = x_1 x_2 \eta m_B^2, \] (A12)

\[ \beta_a = x_2 \eta m_B^2, \] (A13)

\[ \beta_b = x_1 \eta m_B^2, \] (A14)

\[ t_{a(b)} = \max \left( \sqrt{\beta_{a(b)}}, \frac{1}{b_1}, \frac{1}{b_2} \right), \] (A15)

where \( I_0 \) and \( K_0 \) are Bessel functions. The expression of \( s(x, b, Q) \) can be found in Ref.[23]. \( \gamma_q = -\frac{\alpha_s}{\pi} \) is the quark anomalous dimension. \( \alpha_g \) and \( \beta_{a(b)} \) are the virtualities of gluon and quarks, respectively.

**Appendix B: The amplitudes for \( B \to \pi\pi, \pi K, K\bar{K} \) decays**

The amplitude of \( B \) meson nonleptonic weak decay is written as

\[ A(\bar{B} \to M_1 M_2) = \langle M_1 M_2 | \mathcal{H}_{\text{eff}} | \bar{B} \rangle, \] (B1)

where \( \mathcal{H}_{\text{eff}} \) is given in Eq.(1).

The explicit expressions for specific final states are written as

\[ A(B_u^- \to \pi^- \pi^0) \]
\[ \frac{G_F}{2} V_{ub} V_{\ast}^{\dagger} \left\{ a_2 A_{ab}^{LL}(\pi^-, \pi^0) + C_1 A_{cd}^{LL}(\pi^-, \pi^0) + a_1 A_{ab}^{LL}(\pi^0, \pi^-) + C_2 A_{cd}^{LL}(\pi^0, \pi^-) \right\} \\
- \frac{G_F}{2} V_{tb} V_{\ast}^{\dagger} \left\{ \frac{3}{2} (a_9 - a_7) A_{ab}^{LL}(\pi^-, \pi^0) + \frac{1}{2} a_{10} A_{ab}^{LL}(\pi^-, \pi^0) + \frac{1}{2} a_8 A_{ab}^{SP}(\pi^-, \pi^0) + \frac{1}{2} C_9 A_{cd}^{LL}(\pi^-, \pi^0) + \frac{3}{2} C_{10} A_{cd}^{LL}(\pi^-, \pi^0) + \frac{3}{2} C_8 A_{cd}^{LR}(\pi^-, \pi^0) + \frac{1}{2} C_7 A_{cd}^{SP}(\pi^-, \pi^0) + a_{10} A_{ab}^{LL}(\pi^0, \pi^-) + a_8 A_{ab}^{SP}(\pi^0, \pi^-) + C_9 A_{cd}^{LL}(\pi^0, \pi^-) + C_7 A_{cd}^{SP}(\pi^0, \pi^-) \right\}, \quad (B2) \]

\[ \mathcal{A}(B_u^- \rightarrow \pi^- \bar{K}^0) \]

\[ = \frac{G_F}{\sqrt{2}} V_{ub} V_{\ast}^{\dagger} \left\{ a_1 A_{ef}^{LL}(\bar{K}, \pi) + C_2 A_{gh}^{LL}(\bar{K}, \pi) \right\} \]

\[ - \frac{G_F}{\sqrt{2}} V_{tb} V_{\ast}^{\dagger} \left\{ (a_4 - \frac{1}{2} a_{10}) A_{ab}^{LL}(\pi, \bar{K}) + (a_6 - \frac{1}{2} a_8) A_{ab}^{SP}(\pi, \bar{K}) + (C_3 - \frac{1}{2} C_9) A_{cd}^{LL}(\pi, \bar{K}) + (C_5 - \frac{1}{2} C_7) A_{cd}^{SP}(\pi, \bar{K}) \right. \]

\[ + (a_4 + a_{10}) A_{ef}^{LL}(\bar{K}, \pi) + (a_6 + a_8) A_{ef}^{SP}(\bar{K}, \pi) + (C_3 + C_9) A_{gh}^{LL}(\bar{K}, \pi) + (C_5 + C_7) A_{gh}^{SP}(\bar{K}, \pi) \left\}, \quad (B3) \right. \]

\[ \mathcal{A}(B_u^- \rightarrow K^- \pi^0) \]

\[ = \frac{G_F}{2} V_{ub} V_{\ast}^{\dagger} \left\{ a_1 A_{ab}^{LL}(\pi, \bar{K}) + a_2 A_{ab}^{LL}(\bar{K}, \pi) + a_1 A_{ef}^{LL}(\bar{K}, \pi) \right. \]

\[ + C_2 A_{cd}^{LL}(\pi, \bar{K}) + C_1 A_{cd}^{LL}(\bar{K}, \pi) + C_2 A_{gh}^{LL}(\bar{K}, \pi) \left\} \right. \]

\[ - \frac{G_F}{2} V_{tb} V_{\ast}^{\dagger} \left\{ (a_4 + a_{10}) A_{ab}^{LL}(\pi, \bar{K}) + (a_6 + a_8) A_{ab}^{SP}(\pi, \bar{K}) \right. \]

\[ + (C_3 + C_9) A_{cd}^{LL}(\pi, \bar{K}) + (C_5 + C_7) A_{cd}^{SP}(\pi, \bar{K}) \]

\[ + \frac{3}{2} (a_9 - a_7) A_{ab}^{LL}(\bar{K}, \pi) + (a_4 + a_{10}) A_{ef}^{LL}(\bar{K}, \pi) \]

\[ + (a_6 + a_8) A_{ef}^{SP}(\bar{K}, \pi) + \frac{3}{2} C_{10} A_{cd}^{LL}(\bar{K}, \pi) + \frac{3}{2} C_8 A_{cd}^{LR}(\bar{K}, \pi) \]

\[ + (C_3 + C_9) A_{gh}^{LL}(\bar{K}, \pi) + (C_5 + C_7) A_{gh}^{SP}(\bar{K}, \pi) \left\}, \quad (B4) \right. \]

\[ \mathcal{A}(B_u^- \rightarrow K^- K^0) \]

\[ = \frac{G_F}{\sqrt{2}} V_{ub} V_{\ast}^{\dagger} \left\{ a_1 A_{ef}^{LL}(K, \bar{K}) + C_2 A_{gh}^{LL}(K, \bar{K}) \right\} \]

\[ - \frac{G_F}{\sqrt{2}} V_{tb} V_{\ast}^{\dagger} \left\{ (a_4 - \frac{1}{2} a_{10}) A_{ab}^{LL}(\bar{K}, K) + (a_6 - \frac{1}{2} a_8) A_{ab}^{SP}(\bar{K}, K) \right. \]

\[ + (C_3 - \frac{1}{2} C_9) A_{cd}^{LL}(\bar{K}, K) + (C_5 - \frac{1}{2} C_7) A_{cd}^{SP}(\bar{K}, K) \]

\[ + (a_4 + a_{10}) A_{ef}^{LL}(K, \bar{K}) + (a_6 + a_8) A_{ef}^{SP}(K, \bar{K}) \left\}, \quad (B4) \right. \]
\begin{align}
A(B_d^0 \rightarrow \pi^0 \pi^+) &= \frac{G_F}{\sqrt{2}} V_{ub} V_{ud}^* \left\{ a_1 A_{ab}^{LL}(\pi, \pi) + C_2 A_{cd}^{LL}(\pi, \pi) + a_2 A_{ef}^{LL}(\pi, \pi) + C_1 A_{gh}^{LL}(\pi, \pi) \right\} \\
&\quad - \frac{G_F}{\sqrt{2}} V_{tb} V_{td}^* \left\{ (a_4 + a_{10}) A_{ab}^{LL}(\pi, \pi) + (a_6 + a_8) A_{ab}^{SP}(\pi, \pi) + (C_3 + C_9) A_{ab}^{LL}(\pi, \pi) + (C_5 + C_7) A_{ab}^{SP}(\pi, \pi) + (2a_3 + a_4 + 2a_5 + \frac{1}{2}a_7 + \frac{1}{2}a_9 - \frac{1}{2}a_{10}) A_{ef}^{LL}(\pi, \pi) + (a_6 - \frac{1}{2}a_8) A_{ef}^{SP}(\pi, \pi) + (C_3 + 2C_4 - \frac{1}{2}C_9 + \frac{1}{2}C_{10}) A_{gh}^{LL}(\pi, \pi) + (2C_6 + \frac{1}{2}C_8) A_{gh}^{SP}(\pi, \pi) \right\}, \tag{B6}

A(B_d^0 \rightarrow K^- \pi^0) &= - \frac{G_F}{\sqrt{2}} V_{ub} V_{ud}^* \left\{ a_2 (A_{ab}^{LL} - A_{ef}^{LL}) + C_1 (A_{cd}^{LL} - A_{gh}^{LL}) \right\} \\
&\quad - \frac{G_F}{\sqrt{2}} V_{tb} V_{td}^* \left\{ (a_4 + \frac{3}{2}a_7 - \frac{3}{2}a_9 - \frac{1}{2}a_{10}) A_{ab}^{LL} + (a_6 - \frac{1}{2}a_8) (A_{ab}^{SP} + A_{ef}^{SP}) + (C_3 - \frac{1}{2}C_9 - \frac{3}{2}C_{10}) A_{cd}^{LL} - \frac{3}{2}C_8 A_{cd}^{SP} + (C_5 - \frac{1}{2}C_7) (A_{cd}^{SP} + A_{gh}^{SP}) + (2a_3 + a_4 + 2a_5 + \frac{1}{2}a_7 + \frac{1}{2}a_9 - \frac{1}{2}a_{10}) A_{ef}^{LL} + (2C_6 + \frac{1}{2}C_8) A_{gh}^{SP} + (C_3 + 2C_4 - \frac{1}{2}C_9 + \frac{1}{2}C_{10}) A_{gh}^{LL} \right\}, \tag{B7}

A(B_d^0 \rightarrow K^0 \pi^0) &= \frac{G_F}{\sqrt{2}} V_{ub} V_{us}^* \left\{ a_1 A_{ab}^{LL}(\pi, \overline{\pi}) + C_2 A_{cd}^{LL}(\pi, \overline{\pi}) \right\} \\
&\quad - \frac{G_F}{\sqrt{2}} V_{tb} V_{ts}^* \left\{ (a_4 + a_{10}) A_{ab}^{LL}(\pi, \overline{\pi}) + (a_6 + a_8) A_{ab}^{SP}(\pi, \overline{\pi}) + (C_3 + C_9) A_{cd}^{LL}(\pi, \overline{\pi}) + (C_5 + C_7) A_{cd}^{SP}(\pi, \overline{\pi}) + (a_4 - \frac{1}{2}a_{10}) A_{ef}^{LL}(\overline{\pi}, \pi) + (a_6 - \frac{1}{2}a_8) A_{ef}^{SP}(\overline{\pi}, \pi) + (C_3 - \frac{1}{2}C_9) A_{gh}^{LL}(\overline{\pi}, \pi) + (C_5 - \frac{1}{2}C_7) A_{gh}^{SP}(\overline{\pi}, \pi) \right\}, \tag{B8}

A(B_d^0 \rightarrow K^0 \pi^0) &= \frac{G_F}{2} V_{ub} V_{us}^* \left\{ a_2 A_{ab}^{LL}(\overline{\pi}, \pi) + C_1 A_{cd}^{LL}(\overline{\pi}, \pi) \right\}.
\end{align}
\[ + \frac{G_F}{2} V_{tb} V^{*}_{ts} \left\{ (a_4 - \frac{1}{2} a_{10}) A_{ab}^{LL}(\pi, K) + (a_6 - \frac{1}{2} a_8) A_{ab}^{SP}(\pi, K) \\
+ \frac{3}{2} (a_7 - a_9) A_{ab}^{LL}(K, \pi) + (a_4 - \frac{1}{2} a_{10}) A_{cf}^{LL}(K, \pi) \\
+ (a_6 - \frac{1}{2} a_8) A_{cf}^{SP}(K, \pi) + (C_3 - \frac{1}{2} C_9) A_{cd}^{LL}(\pi, K) \\
+ (C_5 - \frac{1}{2} C_7) A_{cd}^{SP}(\pi, K) - \frac{3}{2} C_8 A_{cd}^{LR}(K, \pi) - \frac{3}{2} C_{10} A_{cd}^{LL}(K, \pi) \\
+ (C_3 - \frac{1}{2} C_9) A_{gh}^{LL}(K, \pi) + (C_5 - \frac{1}{2} a_7) A_{gh}^{SP}(K, \pi) \right\}, \quad (B9) \]

\[ \mathcal{A}(B^0_d \to K^- K^+) = \frac{G_F}{\sqrt{2}} V_{ub} V^{*}_{ud} \left\{ a_2 A_{cf}^{LL}(K, \bar{K}) + C_1 A_{gh}^{LL}(K, \bar{K}) \right\} \]

\[- \frac{G_F}{\sqrt{2}} V_{tb} V^{*}_{td} \left\{ (a_3 + a_5 + a_7 + a_9) A_{cf}^{LL}(K, \bar{K}) \\
+ (a_3 + a_5 - \frac{1}{2} a_7 - \frac{1}{2} a_9) A_{cf}^{LL}(\bar{K}, K) \\
+ (C_4 + C_{10}) A_{gh}^{LL}(K, \bar{K}) + (C_6 + C_8) A_{gh}^{LR}(K, \bar{K}) \\
+ (C_4 - \frac{1}{2} C_{10}) A_{gh}^{LL}(\bar{K}, K) + (C_6 - \frac{1}{2} C_8) A_{gh}^{LR}(\bar{K}, K) \right\}, \quad (B10) \]

\[ \mathcal{A}(B^0_d \to \bar{K}^0 K^0) = - \frac{G_F}{\sqrt{2}} V_{tb} V^{*}_{td} \left\{ (a_4 - \frac{1}{2} a_{10}) A_{ab}^{LL}(\bar{K}, K) + (a_6 - \frac{1}{2} a_8) A_{ab}^{SP}(\bar{K}, K) \\
+ (C_3 - \frac{1}{2} C_9) A_{cd}^{LL}(\bar{K}, K) + (C_5 - \frac{1}{2} C_7) A_{cd}^{SP}(\bar{K}, K) \\
+ (a_3 + a_5 - \frac{1}{2} a_7 - \frac{1}{2} a_9) A_{cf}^{LL}(\bar{K}, K) + (C_4 - \frac{1}{2} C_{10}) A_{gh}^{LL}(\bar{K}, K) \\
+ (C_6 - \frac{1}{2} C_8) A_{gh}^{LR}(\bar{K}, K) + (a_6 - \frac{1}{2} a_8) A_{cf}^{SP}(K, \bar{K}) \\
+ (C_3 + C_4 - \frac{1}{2} C_9 - \frac{1}{2} C_{10}) A_{gh}^{LL}(K, \bar{K}) \\
+ (C_6 - \frac{1}{2} C_8) A_{gh}^{LR}(K, \bar{K}) + (C_5 - \frac{1}{2} C_7) A_{gh}^{SP}(K, \bar{K}) \right\}. \quad (B11) \]

The shorthands are

\[ a_i = \begin{cases} C_i + \frac{1}{N_c} C_{i+1}, & \text{for odd } i; \\ C_i - \frac{1}{N_c} C_{i-1}, & \text{for even } i, \end{cases} \quad (B12) \]

\[ C_m A_{ij}^k(M_1, M_2) = i \mathcal{K} \frac{\pi C_F}{N_c^2} m_D^4 f_B f_{M_1} f_{M_2} \left\{ A_i^k(C_m, M_1, M_2) + A_j^k(C_m, M_1, M_2) \right\}, \quad (B13) \]
where the factor $\mathcal{K} = N_c$ for factorizable amplitudes with $ij = ab$ and $ef$, and $\mathcal{K} = 1$ for nonfactorizable amplitudes with $ij = cd$ and $gh$. The expressions of amplitude building block $\mathcal{A}^i_t(C_m, M_1, M_2)$ are given in Appendix C.

**Appendix C: Amplitude building blocks**

There should be a Sudakov factor corresponding to each WF with the pQCD approach. For the sake of convenience in writing, the shorthands such as $\phi_{B1} = \phi_{B1}(x_1, b_1) e^{-S_B}$, $\phi_{B2} = \phi_{B2}(x_1, b_1) e^{-S_B}$, $\phi_M^a = \phi_M^a(x) e^{-S_M}$, $\phi_M^{a'} = \phi_M^{a'}(x) e^{-S_{M'}}$, $\phi_M^{p,t} = r_M \phi_M^{p,t}(x) e^{-S_M}$, $\phi_M^{p,t} = r_M \phi_M^{p,t}(x) e^{-S_{M'}}$ and $\mathcal{A}^i_t = \mathcal{A}^i_t(C_m, M, M')$ will be used in this section. As to the amplitude building block $\mathcal{A}^i_t$, the subscript $i$ corresponds to the indices of Fig.7, and the superscript $j$ refers to the three possible Dirac structures $\Gamma_1 \otimes \Gamma_2$ of the operator $(q_1 q_2)_{\Gamma_1} (\bar{q}_3 q_4)_{\Gamma_2}$, namely $j = LL$ for $(V - A) \otimes (V - A)$, $j = LR$ for $(V - A) \otimes (V + A)$ and $j = SP$ for $-2 (S - P) \otimes (S + P)$. The expressions of $\mathcal{A}^i_t$ are written as follows.

$$\mathcal{A}_a^{LL} = \int dx_1 dx_2 db_1 db_2 C_i(t_a) \alpha_s(t_a) S_1(x_2) H_{ab}(\alpha_g, \beta_a, b_1, b_2)
\{\phi_{B1} [\phi_M^a (1 + x_2) + (\phi_M^p + \phi_M^{a'}) (\bar{x}_2 - x_2)] \\
- \phi_{B2} [\phi_M^a - (\phi_M^p + \phi_M^{a'}) x_2]\},$$  \hspace{1cm} (C1)

$$\mathcal{A}_a^{LR} = -\mathcal{A}_a^{LL},$$  \hspace{1cm} (C2)

$$\mathcal{A}_a^{SP} = 2 r_{M'} \int dx_1 dx_2 db_1 db_2 C_i(t_a) \alpha_s(t_a) S_1(x_2) H_{ab}(\alpha_g, \beta_a, b_1, b_2)
\{\phi_{B1} [\phi_M^a + \phi_M^{p} (2 + x_2) - \phi_M^{a'} x_2] - \phi_{B2} [\phi_M^a + \phi_M^{p} - \phi_M^{a'}]\},$$  \hspace{1cm} (C3)

$$\mathcal{A}_b^{LL} = 2 \int dx_1 dx_2 db_1 db_2 C_i(t_b) \alpha_s(t_b) S_1(x_1) H_{ab}(\alpha_g, \beta_b, b_2, b_1) \phi_{B1} \phi_M^p,$$  \hspace{1cm} (C4)

$$\mathcal{A}_b^{LR} = -\mathcal{A}_b^{LL},$$  \hspace{1cm} (C5)

$$\mathcal{A}_b^{SP} = \int dx_1 dx_2 db_1 db_2 C_i(t_b) \alpha_s(t_b) S_1(x_1) H_{ab}(\alpha_g, \beta_b, b_2, b_1)
2 r_{M'} \{\phi_{B1} [\phi_M^a x_1 + 2 \phi_M^{p} \bar{x}_1] + 2 \phi_{B2} \phi_M^{a'} x_1\},$$  \hspace{1cm} (C6)

$$\mathcal{A}_c^{LL} = \int dx_1 dx_2 dx_3 db_2 db_3 C_i(t_c) \alpha_s(t_c) S_1(x_2) H_{cd}(\alpha_g, \beta_c, b_2, b_3) \phi_M^a
\{ (\phi_{B1} - \phi_{B2}) \phi_M^a (\bar{x}_3 - x_1) - \phi_{B1} (\phi_M^{p} - \phi_M^{a'}) x_2\}_{b_1 = b_2},$$  \hspace{1cm} (C7)
\[ A_{c}^{LR} = \int dx_1 \, dx_2 \, dx_3 \, db_2 \, db_3 \, C_i(t_c) \, \alpha_s(t_c) \, S_i(x_2) \, H_{cd}(\alpha_g, \beta_c, b_2, b_3) \, \phi_M^a \]
\[
\left\{ \left( \phi_B^1 - \phi_B^2 \right) \left[ \phi_M^a (x_1 - \bar{x}_3) + \left( \phi_M^p + \phi_M^l \right) x_2 \right] - \phi_B^1 \, \phi_M^a \, x_2 \right\}_{b_1 = b_2}, \quad (C8)
\]
\[ A_{c}^{SP} = \int dx_1 \, dx_2 \, dx_3 \, db_2 \, db_3 \, C_i(t_c) \, \alpha_s(t_c) \, S_i(x_2) \, H_{cd}(\alpha_g, \beta_c, b_2, b_3) \]
\[
\left\{ \left( \phi_B^1 - \phi_B^2 \right) \left[ \phi_M^a (x_1 - \bar{x}_3) + \left( \phi_M^p + \phi_M^l \right) x_2 \right] - \phi_B^1 \, \phi_M^a \, x_2 \right\}_{b_1 = b_2}, \quad (C9)
\]
\[ A_{d}^{LR} = \int dx_1 \, dx_2 \, dx_3 \, db_2 \, db_3 \, C_i(t_d) \, \alpha_s(t_d) \, S_i(x_2) \, H_{cd}(\alpha_g, \beta_d, b_2, b_3) \, \phi_M^a \]
\[
\left\{ \left( \phi_B^1 - \phi_B^2 \right) \phi_M^a (x_3 - x_1) - \phi_B^1 \left( \phi_M^p - \phi_M^l \right) x_2 \right\}_{b_1 = b_2}, \quad (C10)
\]
\[ A_{d}^{SP} = \int dx_1 \, dx_2 \, dx_3 \, db_2 \, db_3 \, C_i(t_d) \, \alpha_s(t_d) \, S_i(x_2) \, H_{cd}(\alpha_g, \beta_d, b_2, b_3) \, \phi_M^a \]
\[
\left\{ \left( \phi_B^1 - \phi_B^2 \right) \phi_M^a (x_3 - x_1) - \phi_B^1 \left( \phi_M^p - \phi_M^l \right) x_2 \right\}_{b_1 = b_2}, \quad (C11)
\]
\[ A_{e}^{SP} = \int dx_2 \, dx_3 \, db_2 \, db_3 \, C_i(t_e) \, \alpha_s(t_e) \, S_i(\bar{x}_3) \, H_{ef}(\omega_g, \beta_e, b_2, b_3) \]
\[
\left\{ \phi_M^a \, \phi_M^a \, \bar{x}_3 + 2 \phi_M^p \left[ \phi_{M'}^p (1 + \bar{x}_3) + \phi_{M'}^l \, \bar{x}_3 \right] \right\}, \quad (C13)
\]
\[
A_{c}^{LR} = + A_{c}^{LL}, \quad (C14)
\]
\[ A_{e}^{SP} = \int dx_2 \, dx_3 \, db_2 \, db_3 \, C_i(t_e) \, \alpha_s(t_e) \, S_i(\bar{x}_3) \, H_{ef}(\omega_g, \beta_e, b_2, b_3) \]
\[
\left\{ \phi_M^a \, \phi_M^a \, \bar{x}_3 + 2 \phi_M^p \left[ \phi_{M'}^p (1 + \bar{x}_3) + \phi_{M'}^l \, \bar{x}_3 \right] \right\}, \quad (C15)
\]
\[ A_{f}^{LR} = + A_{f}^{LL}, \quad (C17)
\]
\[ A_{f}^{SP} = \int dx_2 \, dx_3 \, db_2 \, db_3 \, C_i(t_f) \, \alpha_s(t_f) \, S_i(x_2) \, H_{ef}(\omega_g, \beta_f, b_3, b_2) \]
\[ \mathcal{A}^{LL}_g = \int dx_1 dx_2 dx_3 db_1 db_2 C_i(t_g) \alpha_s(t_g) H_{gh}(\omega_g, \beta_g, b_1, b_2) \]
\[ \{ \phi_{B2} (\phi^p_M - \phi^t_M) [\phi^p_{M'} (x_1 + x_3 + 1) + \phi^t_{M'} (x_1 - x_3)] \]
\[ - \phi_{B1} [\phi^a_M \phi^a_{M'} x_2 + 2 \phi^p_M \phi^t_{M'} (1 + x_2) + 2 \phi^t_M \phi^t_{M'} \bar{x}_2 \]
\[ + (\phi^p_M - \phi^t_M) (\phi^p_{M'} + \phi^t_{M'}) (x_1 - x_2 + \bar{x}_3) \} \}_{b_2=b_3}, \quad (C19) \]

\[ \mathcal{A}^{LR}_g = - \int dx_1 dx_2 dx_3 db_1 db_2 C_i(t_g) \alpha_s(t_g) H_{gh}(\omega_g, \beta_g, b_1, b_2) \]
\[ \{ (\phi_{B1} - \phi_{B2}) \phi^a_M \phi^a_{M'} (x_1 + \bar{x}_3) + \phi_{B1} [2 \phi^p_M \phi^t_{M'} (1 + x_2) \]
\[ + 2 \phi^t_M \phi^t_{M'} \bar{x}_2 + (\phi^p_M + \phi^t_M) (\phi^p_{M'} - \phi^t_{M'}) (x_1 - x_2 + \bar{x}_3) \]
\[ - \phi_{B2} (\phi^p_{M'} - \phi^t_{M'}) [\phi^p_M (x_1 + \bar{x}_3 + 1) + \phi^t_M (x_1 - x_3)] \} \}_{b_2=b_3}, \quad (C20) \]

\[ \mathcal{A}^{SP}_g = \int dx_1 dx_2 dx_3 db_1 db_2 C_i(t_g) \alpha_s(t_g) H_{gh}(\omega_g, \beta_g, b_1, b_2) \]
\[ \{ \phi_{B1} [\phi^a_M (\phi^a_{M'} - \phi^t_{M'}) (x_1 + \bar{x}_3 - 2) + \phi^a_{M'} (\phi^p_M + \phi^t_M) (2 - x_2)] \]
\[ - \phi_{B2} [\phi^a_M (\phi^p_{M'} - \phi^t_{M'}) (x_1 - x_3) + \phi^a_{M'} (\phi^p_M + \phi^t_M)] \} \}_{b_2=b_3}, \quad (C21) \]

\[ \mathcal{A}^{LL}_h = \int dx_1 dx_2 dx_3 db_1 db_2 C_i(t_h) \alpha_s(t_h) H_{gh}(\omega_g, \beta_h, b_1, b_2) \]
\[ \{ (\phi_{B1} - \phi_{B2}) (\bar{x}_3 - x_1) [\phi^a_M \phi^a_{M'} + (\phi^p_M + \phi^t_M) (\phi^p_{M'} - \phi^t_{M'})] \]
\[ + \phi_{B1} x_2 (\phi^p_M - \phi^t_M) (\phi^p_{M'} + \phi^t_{M'}) \} \}_{b_2=b_3}, \quad (C22) \]

\[ \mathcal{A}^{LR}_h = \int dx_1 dx_2 dx_3 db_1 db_2 C_i(t_h) \alpha_s(t_h) H_{gh}(\omega_g, \beta_h, b_1, b_2) \]
\[ \{ (\phi_{B1} - \phi_{B2}) (\bar{x}_3 - x_1) (\phi^p_M - \phi^t_M) (\phi^p_{M'} + \phi^t_{M'}) \]
\[ + \phi_{B1} x_2 [\phi^a_M \phi^a_{M'} + (\phi^p_M + \phi^t_M) (\phi^p_{M'} - \phi^t_{M'})] \} \}_{b_2=b_3}, \quad (C23) \]

\[ \mathcal{A}^{SP}_h = \int dx_1 dx_2 dx_3 db_1 db_2 C_i(t_h) \alpha_s(t_h) H_{gh}(\omega_g, \beta_h, b_1, b_2) \]
\[ \{ \phi_{B1} [x_2 \phi^a_{M'} (\phi^p_{M'} + \phi^t_{M'}) + (x_1 - \bar{x}_3) \phi^a_M (\phi^p_{M'} - \phi^t_{M'})] \]
\[ - \phi_{B2} x_2 \phi^a_{M'} (\phi^p_M + \phi^t_M) \} \}_{b_2=b_3}, \quad (C24) \]

\[ H_{cd}(\alpha, \beta, b_i, b_j) = b_i b_j \{ \theta(b_i - b_j) K_0(b_i \sqrt{\alpha}) I_0(b_j \sqrt{\alpha}) + (b_i \leftrightarrow b_j) \} K_0(b_j \sqrt{\beta}), \quad (C25) \]
\[ H_{ef}(\omega, \beta, b_i, b_j) = -\frac{\pi^2}{4} b_i b_j \left\{ \theta(b_i - b_j) \left[ J_0(b_i\sqrt{\beta}) + i Y_0(b_i\sqrt{\beta}) \right] J_0(b_j\sqrt{\beta}) \\
+ (b_i \leftrightarrow b_j) \right\} \left\{ J_0(b_i\sqrt{\omega}) + i Y_0(b_i\sqrt{\omega}) \right\}, \quad (C26) \]

\[ H_{gh}(\omega, \beta, b_i, b_j) = i \frac{\pi}{2} b_i b_j \left\{ \left[ J_0(b_i\sqrt{\omega}) + i Y_0(b_i\sqrt{\omega}) \right] J_0(b_j\sqrt{\omega}) + (b_i \leftrightarrow b_j) \right\} \left\{ i \frac{\pi}{2} \theta(\beta) \left[ J_0(b_i\sqrt{\beta}) + i Y_0(b_i\sqrt{\beta}) \right] + \theta(-\beta) K_0(b_i\sqrt{-\beta}) \right\}, \quad (C27) \]

\[ \alpha_g = x_1 x_2 m_B^2, \quad (C28) \]
\[ \omega_g = x_2 \bar{x}_3 m_B^2, \quad (C29) \]
\[ \beta_a = x_2 m_B^2, \quad (C30) \]
\[ \beta_b = x_1 m_B^2, \quad (C31) \]
\[ \beta_c = x_2 (x_1 - \bar{x}_3) m_B^2, \quad (C32) \]
\[ \beta_d = x_2 (x_1 - x_3) m_B^2, \quad (C33) \]
\[ \beta_e = \bar{x}_3 m_B^2, \quad (C34) \]
\[ \beta_f = x_2 m_B^2, \quad (C35) \]
\[ \beta_g = (x_2 \bar{x}_3 - \bar{x}_1 x_2 - \bar{x}_3) m_B^2, \quad (C36) \]
\[ \beta_h = x_2 (\bar{x}_3 - x_1) m_B^2, \quad (C37) \]
\[ t_i = \max \left( \frac{1}{b_1}, \frac{1}{b_2}, \sqrt{\beta_i} \right), \text{ for } i = a, b; \quad (C38) \]
\[ t_i = \max \left( \frac{1}{b_2}, \frac{1}{b_3}, \sqrt{\beta_i} \right), \text{ for } i = c, d; \quad (C39) \]
\[ t_i = \max \left( \frac{1}{b_2}, \frac{1}{b_3}, \sqrt{\beta_i} \right), \text{ for } i = e, f; \quad (C40) \]
\[ t_i = \max \left( \frac{1}{b_1}, \frac{1}{b_2}, \sqrt{\omega_g}, \sqrt{\beta_i} \right), \text{ for } i = g, h. \quad (C41) \]

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