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Towards a precision determination of α in $B \to \pi\pi$ decays

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An assumption of isospin symmetry permits the determination of $\sin(2\alpha)$ from the experimental study of $B \to \pi\pi$ decays. Isospin, however, is merely an approximate symmetry; its breaking predicates a theoretical systematical error $\sigma_\alpha^{\rm IB}$ in the extraction of α. We focus on the impact of $\pi^0 - \eta$, η' mixing, as well as the manner in which it is amenable to empirical constraint, and determine that $\sigma_\alpha^{\rm IB}$ can potentially be controlled to $\mathcal{O}(1^\circ)$.

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I. INTRODUCTION

Probing the mechanism of CP violation in the B-meson system demands that the angles of the unitarity triangle, α, β, and γ, be extracted a plurality of ways [1]. The study of $B \to \pi\pi$ decays, e.g., permits the determination of $\sin(2\alpha)$, where $\alpha \equiv \phi_2 \equiv \mathrm{Arg}(-V_{tb}^* V_{td}/V_{ub}^* V_{ud})$ and we recall that $\alpha + \beta + \gamma = \pi (\mathrm{mod} 2\pi)$ in the standard model [2]. The measurement of the time-dependent, CP-violating asymmetries in $B, \bar{B} \to \pi^+\pi^-$ decays determine $S_{\pi\pi}$ and $C_{\pi\pi}$; these measurements in themselves determine $\sin(2\alpha_{\rm eff})$, where

$$\sin(2\alpha_{\rm eff}) = \frac{S_{\pi\pi}}{\sqrt{1 - C_{\pi\pi}^2}}. \tag{1}$$

Penguin contributions make the parameter $\alpha_{\rm eff}$ differ from α. Gronau and London have noted, however, that the "pollution" $\Delta\alpha \equiv \alpha_{\rm eff} - \alpha$ can be determined and removed with additional $B, \bar{B} \to \pi\pi$ data under an assumption of isospin symmetry [3]. Isospin is an approximate symmetry—the u and d quarks differ in both their charge and mass; such isospin-breaking effects make the determination of $\Delta\alpha$ imperfect. It is our purpose to study these effects, to the end of assessing the irreducible theoretical error $\sigma_\alpha^{\rm IB}$ in the determination of $\Delta\alpha$ via this method. Such is crucial to precision tests of the standard model of CP violation, realized through improved measurements at the current B-meson factories and beyond [4]. Earlier work has focused on the impact of $|\Delta I| = 3/2$ electroweak penguins [5] and on the role of $\pi^0 - \eta$, η' mixing on $\Delta\alpha$ [6]. The treatment of the latter, due to Gardner [6], has recently been reexamined by Gronau and Zupan [7]. The purpose of this article is to amend that work [7] and to update the analysis of Ref. [6].

II. ISOSPIN ANALYSIS IN $B \to \pi\pi$ DECAY

We begin by reviewing the isospin analysis in the isospin-perfect limit [3]. In this limit, the π^+, π^0, and π^- mesons form a degenerate isospin triplet, and the $B \to \pi^+\pi^-$ decay amplitude must be symmetric under the exchange of the two pions, as per the constraint of Bose symmetry. We can relate the two-pion states to states of definite isospin I, $|(\pi\pi)_I\rangle$, via

$$\begin{aligned} |\pi^+\pi^-\rangle &\propto |(\pi\pi)_0\rangle + \frac{1}{\sqrt{2}}|(\pi\pi)_2\rangle \\ |\pi^0\pi^0\rangle &\propto |(\pi\pi)_0\rangle - \sqrt{2}|(\pi\pi)_2\rangle, \end{aligned} \tag{2}$$

where the properly symmetrized state is $|\pi^-\pi^+\rangle_{\rm sym} \equiv (|\pi_1^+\pi_2^-\rangle + |\pi_1^-\pi_2^+\rangle)/\sqrt{2} = \sqrt{2}|\pi^+\pi^-\rangle$ [8]. The particles of the $\pi^0\pi^0$ final state are identical, so that this state need not be symmetrized—if symmetrization is performed nevertheless, an additional factor of $1/2$ must be applied to yield the correct branching ratio. The $B^-, \bar{B}^0$ form a degenerate isospin doublet as well; evaluating the Clebsch-Gordon coefficients allows us to write a decomposition in terms of amplitudes A_I of definite isospin [8]:

$$\begin{aligned} A_{B^0\to\pi^+\pi^-} &\equiv \langle\pi^+\pi^-|\mathcal{H}_W|B^0\rangle \equiv A_0 + \frac{1}{\sqrt{2}}A_2, \\ A_{B^0\to\pi^0\pi^0} &\equiv \langle\pi^0\pi^0|\mathcal{H}_W|B^0\rangle \equiv A_0 - \sqrt{2}A_2, \\ A_{B^+\to\pi^+\pi^0} &\equiv \langle\pi^+\pi^0|\mathcal{H}_W|B^+\rangle \equiv \frac{3}{2}A_2, \end{aligned} \tag{3}$$

where analogous relationships in the charge-conjugate modes ($\bar{A}$) are implied. We recall that A_0 and A_2 are generated by $|\Delta I| = 1/2$ and $|\Delta I| = 3/2$ weak transitions, respectively. Since the symmetrized states $|\pi^-\pi^+\rangle_{\rm sym}$ and $|\pi^+\pi^0\rangle_{\rm sym}$ appear in the physical amplitudes, the $B \to \pi^+\pi^-$ and $B \to \pi^+\pi^0$ partial widths are a factor of 2 larger than suggested by Eq. (3) [9]. We note that the reduced transition rate $\gamma(B \to \pi_1\pi_2)$ is related to the partial width $\Gamma(B \to \pi_1\pi_2)$ via

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$$\Gamma(B\to\pi_1\pi_2)\equiv\frac{1}{16\pi M_B}\sqrt{\left(1-\frac{(M_{\pi_1}+M_{\pi_2})^2}{M_B^2}\right)\left(1-\frac{(M_{\pi_1}-M_{\pi_2})^2}{M_B^2}\right)}\gamma(B\to\pi_1\pi_2). \quad (4)$$

Employing experimental masses throughout, we find, in specific,

$$\gamma_{+-}\equiv\gamma(B\to\pi^+\pi^-)=2|A_{B\to\pi^+\pi^-}|^2,$$
$$\gamma_{+0}\equiv\gamma(B^+\to\pi^+\pi^0)=2|A_{B^+\to\pi^+\pi^0}|^2, \quad (5)$$
$$\gamma_{00}\equiv\gamma(B\to\pi^0\pi^0)=|A_{B\to\pi^0\pi^0}|^2.$$

We note that electromagnetic radiative corrections, which may well be important, should be applied to yield the empirical decay widths and ultimately the reduced transition rates [10]. Irrespective of such corrections, if we rewrite the amplitudes of Eq. (3), which satisfy the "triangle relation,"

$$\frac{1}{\sqrt{2}}(A_{B\to\pi^+\pi^-}-A_{B\to\pi^0\pi^0})=A_{B^+\to\pi^+\pi^0}, \quad (6)$$

in terms of the amplitudes

$$A_{+-}\equiv\sqrt{2}A_{B\to\pi^+\pi^-},\qquad A_{00}\equiv -A_{B\to\pi^0\pi^0},$$
$$A_{+0}\equiv\sqrt{2}A_{B^+\to\pi^+\pi^0}, \quad (7)$$

defined so that $|A_{ij}|=\sqrt{\gamma_{ij}}$, we find

$$A_{+-}+\sqrt{2}A_{00}=\sqrt{2}A_{+0}. \quad (8)$$

We assume $\sqrt{2}|A_2|\geq|A_0|$, so that $\mathrm{Re}A_{B\to\pi^0\pi^0}\leq 0$. This assumption is consistent with theoretical assays of $B\to\pi\pi$ decay in an operator product expansion framework [11], as well as with the pattern of empirical branching ratios, given current errors [12]. Note that a similar triangle relation holds for the charge-conjugate modes and thus

$$\bar{A}_{+-}+\sqrt{2}\bar{A}_{00}=\sqrt{2}\bar{A}_{-0}, \quad (9)$$

where we note $|\bar{A}_{-0}|^2\equiv\gamma(B^-\to\pi^-\pi^0)$. The form of Eqs. (8) and (9) is identical to that of earlier analyses [3,6,7], once differing definitions are taken into account. The upshot of the isospin analysis is that the shift of $\alpha_{\rm eff}$ from α induced by the penguin amplitude in $B\to\pi^+\pi^-$, namely

$$\Delta\alpha\equiv\alpha_{\rm eff}-\alpha\equiv\tfrac{1}{2}\mathrm{Arg}(e^{2i\gamma}\bar{A}_{+-}A^*_{+-}), \quad (10)$$

can be expressed in terms of empirically determined quantities. In particular, with $\phi\equiv\mathrm{Arg}(A_{+-}A^*_{+0})$ and $\bar{\phi}\equiv\mathrm{Arg}(\bar{A}_{+-}\bar{A}^*_{-0})$, we have [3,7]

$$\Delta\alpha_{\rm isospin}\equiv\tfrac{1}{2}(\bar{\phi}-\phi)$$
$$=\tfrac{1}{2}(\mathrm{Arg}(e^{2i\gamma}\bar{A}_{+-}A^*_{+-})-\mathrm{Arg}(e^{2i\gamma}\bar{A}_{-0}A^*_{+0})). \quad (11)$$

In the isospin-perfect limit, as we examine here, $A_{+0}=\exp(2i\gamma)\bar{A}_{-0}$, so that the second term vanishes and $\Delta\alpha_{\rm isospin}=\Delta\alpha$. Geometrically this implies that the two triangles share a common side; namely, $\sqrt{\gamma_{+0}}=\sqrt{\bar{\gamma}_{-0}}$. Let us now turn to an analysis of isospin-breaking effects. Interestingly, the most significant uncertainty arises from the manner in which $\Delta\alpha_{\rm isospin}\neq\Delta\alpha$, promoting the importance of direct theoretical assays of $\Delta\alpha$ [13].

III. ISOSPIN BREAKING IN $B\to\pi\pi$ DECAY

The charge and mass of the up and down quarks do differ, so that the predictions of the isospin analysis we have discussed cannot strictly hold. There are two different effects to consider. Firstly, penguin contributions of $|\Delta I|=3/2$ character can occur, mediated either by electroweak penguin effects, or by isospin breaking in the strong-penguin matrix elements [6,14,15]. Secondly, the triangle relationships of Eqs. (8) and (9) need no longer hold [6]. For example, the physical, neutral-pion state contains isoscalar components due to mixing with the η and η', engendering an "$I=1$" amplitude in $B\to\pi\pi$ decay [6]. The η and η' admixtures in the π^0 are generated by the strong interaction in $\mathcal{O}(m_d-m_u)$. Alternatively, we can regard this interaction as an $I=1$ "spurion," encoding isospin-violating effects so that the matrix elements with the spurion are $\mathrm{SU}(2)_f$ invariant [16]. In this latter picture, the "extra" amplitude engendered by $\pi^0-\eta,\eta'$ mixing can be recast as a $|\Delta I|=5/2$ amplitude, generated by $\mathcal{O}(m_d-m_u)$ or $\mathcal{O}(\alpha)$ effects in concert with a $|\Delta I|=3/2$ weak transition. A $|\Delta I|=5/2$ transition can also be realized by isospin-breaking effects in concert with a $|\Delta I|=1/2$ weak transition [9], though, as per the spurion picture, such is not engendered by $\pi^0-\eta,\eta'$ mixing in leading order in isospin breaking. Writing $A_{|\Delta I|,I}$, we replace Eq. (3) with [8,17]

$$A_{B^0\to\pi^+\pi^-}\equiv A_{1/2,0}+\frac{1}{\sqrt{2}}(A_{3/2,2}-A_{5/2,2}),$$
$$A_{B^0\to\pi^0\pi^0}\equiv A_{1/2,0}-\sqrt{2}(A_{3/2,2}-A_{5/2,2}), \quad (12)$$
$$A_{B^+\to\pi^+\pi^0}\equiv\frac{3}{2}A_{3/2,2}+\sqrt{\frac{3}{2}}A_{5/2,2}.$$

We note that this parametrization suffices to capture isospin breaking in $B \to \pi\pi$ decay, as three theoretical amplitudes describe the three empirical ones. Isospin breaking impacts the determination of $\Delta\alpha$ in two distinct ways. For example, it can break the triangle relation, Eq. (6). If the triangle relation is broken in an ill-determined way, the ability to assess the angles ϕ and $\bar{\phi}$ is compromised. If the triangle relation is not broken, however, then the application of the isospin decomposition given in Eq. (3) permits the determination of ϕ and $\bar{\phi}$ *regardless* of whether additional isospin-breaking effects are present. Isospin breaking, however, can also make $\Delta\alpha_{\text{isospin}}$ differ from $\Delta\alpha$; specifically, $\text{Arg}(e^{2i\gamma}\bar{A}_{-0}A^*_{+0}) \neq 0$, recalling Eq. (11). If the impact of both effects can be estimated, if not controlled via empirical constraints, we can assess the irreducible theoretical error in the determination of $\Delta\alpha$. Interpreting these two effects in terms of the parametrization of Eq. (12), a nonzero value of the $A_{5/2,2}$ amplitude signals the breaking of the triangle relation, whereas penguin contributions to $A_{B^+\to\pi^+\pi^0}$, to $A_{3/2,2}$, make $\text{Arg}(e^{2i\gamma}\bar{A}_{-0}A^*_{+0}) \neq 0$ even if $A_{5/2,2} = 0$. Electroweak penguin contributions are an example of the latter effect [18]. Since current experimental data is consistent with $|A_{3/2,2}| \gtrsim |A_{1/2,0}|$ in $B \to \pi\pi$ decay, we expect that $\pi^0 - \eta, \eta'$ mixing will play the most important role in the realization of a $A_{5/2,2}$ amplitude. In the limit that the $A_{5/2,2}$ amplitude is generated exclusively in this manner, $\text{Arg}(e^{2i\gamma}\bar{A}_{-0}A^*_{+0}) \neq 0$ can only be realized through penguin contributions of $|\Delta I| = 3/2$ character. The phenomenon of $\pi^0 - \eta, \eta'$ mixing can generate both effects; let us consider it explicitly.

A. $\pi^0 - \eta, \eta'$ mixing

In what follows we examine the role of $\pi^0 - \eta, \eta'$ mixing on the extraction of α from $B \to \pi\pi$ decays. We distinguish the amplitude for decay to physical pion final states, which suffer $\pi^0 - \eta, \eta'$ mixing, e.g., $A_{B\to\pi^0\pi^0}$, from the amplitude in the isospin-perfect limit, $A_{B\to\phi_3\phi_3}$, where ϕ_3 denotes the isospin-triplet state with $I_3 = 0$. Noting earlier work on $\pi^0 - \eta, \eta'$ mixing in $K \to \pi\pi$ decay [8,19,20], we have

$$\begin{aligned} A_{B^+\to\pi^+\pi^0} &= A_{B^+\to\pi^+\phi_3} + \varepsilon A_{B^+\to\pi^+\eta} + \varepsilon' A_{B^+\to\pi^+\eta'}, \\ A_{B\to\pi^0\pi^0} &= A_{B\to\phi_3\phi_3} + 2\varepsilon A_{B\to\phi_3\eta} + 2\varepsilon' A_{B\to\phi_3\eta'}, \end{aligned} \tag{13}$$

where we assert $\varepsilon, \varepsilon' \sim \mathcal{O}((m_d - m_u)/\Lambda_{\text{had}})$ or $\mathcal{O}(\alpha)$ and neglect all higher-order terms in isospin-breaking parameters. To gain insight on the nature of Λ_{had}, we note that the analysis of the pseudoscalar meson octet in current algebra [21], or in lowest order chiral perturbation theory [22], determine the $\pi^0 - \eta_8$ mixing angle ε_8 to be

$$\varepsilon_8 = \frac{\sqrt{3}}{4}\left(\frac{m_d - m_u}{m_s - \hat{m}}\right), \tag{14}$$

with $\hat{m} = (m_u + m_d)/2$, so that we expect $\Lambda_{\text{had}} \sim \mathcal{O}(m_s)$. The impact of isospin breaking is controlled by the magnitude of $\text{SU}(3)_f$ breaking. The breaking of $\text{SU}(3)_f$ symmetry also engenders the mixing of the pseudoscalar octet and singlet states, η_8 and η_0, to realize the observed η and η' states. Such considerations demand that we evaluate $A_{B\to\pi\eta^{(\prime)}}$ in the presence of $\text{SU}(3)_f$ breaking effects. We postpone specific estimates of ε and ε' to the discussion of our numerical results. We may use these relationships to rewrite the triangle relation, Eq. (6), which now appears as

$$\frac{1}{\sqrt{2}}(A_{B\to\pi^+\pi^-} - A_{B\to\phi_3\phi_3}) = A_{B^+\to\pi^+\phi_3}, \tag{15}$$

in terms of amplitudes employing physical π^0 states. That is,

$$\begin{aligned} \frac{1}{\sqrt{2}}(A_{B\to\pi^+\pi^-} - A_{B\to\pi^0\pi^0}) = A_{B^+\to\pi^+\pi^0} &- \sqrt{2}\varepsilon A_{B\to\phi_3\eta} \\ &- \sqrt{2}\varepsilon' A_{B\to\phi_3\eta'} - \varepsilon A_{B^+\to\pi^+\eta} \\ &- \varepsilon' A_{B^+\to\pi^+\eta'}, \end{aligned} \tag{16}$$

where replacing $A_{B\to\phi_3\eta^{(\prime)}}$ with $A_{B\to\pi^0\eta^{(\prime)}}$ generates corrections of higher order in $\varepsilon, \varepsilon'$, which are negligible in the order to which we work. Note that $\eta^{(\prime)}$ connotes either η or η' throughout. We observe that the triangle relation is broken in the presence of isospin-breaking effects [6].

We turn to theory to assess the impact of the amplitudes containing η, η' on Eq. (16). The QCD factorization approach [23] to hadronic B-meson decay analyzes the decay amplitudes in a systematic expansion in inverse powers of the heavy-quark mass m_b and the strong coupling constant $\alpha_s(\mu)$, where $\mu \sim \mathcal{O}(m_b)$. Crucial to the treatment of the decay amplitudes in this case is that of the physical η and η' states themselves, as the η and η' mix. These states are not simple flavor-octet and flavor-singlet states, as $\text{SU}(3)_f$ symmetry would suggest, but rather each physical state is a mixture of these components. The presence of the flavor-singlet component in decays to $\eta^{(\prime)}$ final states admits novel decay mechanisms, in part mediated by the axial anomaly, not present in other channels [24]. We emphasize, as recognized in Ref. [24], that these flavor-singlet contributions are not captured by the analysis of non-$\eta^{(\prime)}$ decay channels with an assumption of $\text{SU}(3)_f$ symmetry. To implement $\eta - \eta'$ mixing, we employ the Feldmann-Kroll-Stech scheme [25], also adopted in Refs. [24,26], in which a single mixing angle characterizes the decomposition of $|\eta^{(\prime)}\rangle$ into the flavor states $|\eta_q\rangle = (|u\bar{u}\rangle + |d\bar{d}\rangle)/\sqrt{2}$ and $|\eta_s\rangle = |s\bar{s}\rangle$. Beneke and Neubert thus determine [26]

$$\sqrt{2}A^{\rm BN}_{B^-\to\pi^-\eta^{(\prime)}} + 2A^{\rm BN}_{\bar{B}^0\to\phi_3\eta^{(\prime)}} = \sum_{p=u,c}\lambda_p\bigg\{A_{\pi\eta_q^{(\prime)}}[\delta_{pu}(\beta_1+\beta_2+2\beta_{S1}+2\beta_{S2})] + \sqrt{2}A_{\pi\eta_s^{(\prime)}}\bigg[\delta_{pu}(\beta_{S1}+\beta_{S2}) + \frac{3}{2}\beta^p_{S3,\rm EW} + \frac{3}{2}\beta^p_{S4,\rm EW}\bigg] + A_{\eta_q^{(\prime)}\pi}\bigg[\delta_{pu}(\alpha_1+\alpha_2+\beta_1+\beta_2) + \frac{3}{2}\alpha^p_{3,\rm EW} + \frac{3}{2}\alpha^p_{4,\rm EW} + \frac{3}{2}\beta^p_{3,\rm EW} + \frac{3}{2}\beta^p_{4,\rm EW}\bigg]\bigg\}, \tag{17}$$

where $\lambda_p \equiv V_{pb}V^*_{pd}$, and we refer to Ref. [26] for all details. In this expression, the meson masses, decay constants, form factors, and light-cone distribution functions are all evaluated in the isospin-symmetric limit. Note, however, that the physical quark charges have been employed, so that, in particular, $e_u \neq e_d$, in the evaluation of the electroweak penguin contributions. We note that the role of a possible $c\bar{c}$ component in the $\eta^{(\prime)}$ mesons has been included in the computation of $A_{B^-\to\pi^-\eta^{(\prime)}}$ and $A_{\bar{B}^0\to\phi_3\eta^{(\prime)}}$, although such effects are likely most significant in $b\to sq\bar{q}$ transitions [27], which we do not treat here. The amplitudes are computed in next-to-leading order in α_s and at leading power in $\Lambda_{\rm QCD}/m_b$. The terms representing weak annihilation contributions are denoted by "β" and are included, although they are formally suppressed by a power of m_b. The computation of these contributions suffer end-point divergences in QCD factorization, so that their estimate is uncertain. The large direct CP asymmetry found in the penguin-dominated mode $B\to K^+\pi^-$ [12] suggests that annihilation contributions may well play a larger phenomenological role than anticipated [26]. Nevertheless, if we do neglect the annihilation contributions, as they are power-suppressed and largely possess, in this case, the same weak phase as the dominant contributions, we have

$$\sqrt{2}A^{\rm BN}_{B^-\to\pi^-\eta^{(\prime)}} + 2A^{\rm BN}_{\bar{B}^0\to\phi_3\eta^{(\prime)}} = \sum_{p=u,c}\lambda_p\bigg\{A_{\eta_q^{(\prime)}\pi}\bigg[\delta_{pu}(\alpha_1+\alpha_2) + \frac{3}{2}\alpha^p_{3,\rm EW} + \frac{3}{2}\alpha^p_{4,\rm EW}\bigg]\bigg\}, \tag{18}$$

where the α_i implicitly depend on the order of the arguments of the A_{ij} prefactor, so that $\alpha_i^{(p)} \equiv \alpha_i^{(p)}(\eta_q^{(\prime)}\pi)$. By comparison, we note that

$$\sqrt{2}A^{\rm BN}_{B^-\to\pi^-\phi_3} = \sum_{p=u,c}\lambda_p\bigg\{A_{\pi\pi}\bigg[\delta_{pu}(\alpha_1+\alpha_2) + \frac{3}{2}\alpha^p_{3,\rm EW} + \frac{3}{2}\alpha^p_{4,\rm EW}\bigg]\bigg\}, \tag{19}$$

where we emphasize that $\alpha_i^{(p)} \equiv \alpha_i^{(p)}(\pi\pi)$ in this case. The electroweak penguin contributions which appear in this expression are explicitly of $|\Delta I| = 3/2$ character. That is, were the quark-charge dependence made manifest, we would see that these contributions are proportional to $e_u - e_d$, so that, in analogy to our discussion of $\pi^0 - \eta, \eta'$ mixing, the electroweak contribution contains an effective isovector interaction acting in concert with a $|\Delta I| = 1/2$ transition. Thus we can write

$$A^{\rm BN}_{B^-\to\pi^-\eta^{(\prime)}} + \sqrt{2}A^{\rm BN}_{\bar{B}^0\to\phi_3\eta^{(\prime)}} = A^{\rm BN}_{B^-\to\pi^-\phi_3}\bar{X}_{\eta_q^{(\prime)}}, \tag{20}$$

where

$$\bar{X}_{\eta_q^{(\prime)}} = \bigg[\frac{A_{\eta_q^{(\prime)}\pi}}{A_{\pi\pi}}\bigg]\bigg[\frac{\bar{\Sigma}(\eta_q^{(\prime)}\pi)}{\bar{\Sigma}(\pi\pi)}\bigg] \tag{21}$$

and

$$\bar{\Sigma}(M_1M_2) = \sum_{p=u,c}\lambda_p\bigg[\delta_{pu}(\alpha_1+\alpha_2) + \frac{3}{2}\alpha^p_{3,\rm EW} + \frac{3}{2}\alpha^p_{4,\rm EW}\bigg], \tag{22}$$

with $\alpha_i^{(p)} \equiv \alpha_i^{(p)}(M_1M_2)$. We note $A_{B^i\to\pi^j\pi^k} = A^{\rm BN}_{B^i\to\pi^j\pi^k}/\sqrt{2}$, so that the amplitudes $A^{\rm BN}_{B^i\to\pi^j\pi^k}$ satisfy both Eqs. (3) and (6), though the A_I thus determined would be $\sqrt{2}$ larger. Nevertheless, no physics can depend on this normalization choice, so that we must have

$$\frac{|A^{BN}_{B^-\to\pi^-\eta^{(\prime)}}|}{|A^{BN}_{B^-\to\pi^-\phi_3}|} = \frac{|A_{B^-\to\pi^-\eta^{(\prime)}}|}{|A_{B^-\to\pi^-\phi_3}|}, \qquad \frac{|A^{BN}_{\bar{B}^0\to\phi_3\eta^{(\prime)}}|}{|A^{BN}_{\bar{B}^0\to\phi_3\phi_3}|} = \frac{|A_{\bar{B}^0\to\phi_3\eta^{(\prime)}}|}{|A_{\bar{B}^0\to\phi_3\phi_3}|}, \tag{23}$$

as well as

$$A_{B^-\to\pi^-\eta^{(\prime)}} + \sqrt{2}A_{\bar{B}^0\to\phi_3\eta^{(\prime)}} = A_{B^-\to\pi^-\phi_3}\bar{X}_{\eta_q^{(\prime)}}. \tag{24}$$

Returning to Eq. (16), we find

$$\frac{1}{\sqrt{2}}(A_{B\to\pi^+\pi^-} - A_{B\to\pi^0\pi^0}) = (1-\xi)A_{B^+\to\pi^+\pi^0}, \tag{25}$$

where ξ, which need not be real, is given by

$$\xi = \varepsilon[X_{\eta_q} + \ldots] + \varepsilon'[X_{\eta_q'} + \ldots]. \tag{26}$$

We note that $\bar{X}_{\eta_q^{(\prime)}} \xleftrightarrow{CP} X_{\eta_q^{(\prime)}}$, $\bar{\Sigma}(M_1M_2) \xleftrightarrow{CP} \Sigma(M_1M_2)$, and $\lambda_p \xleftrightarrow{CP} \lambda_p^*$ under CP transformation, whereas each ellipsis denotes neglected annihilation corrections. It is worth emphasizing that this result differs from its analogue in Ref. [7] in an important way. That is, we have not assumed $SU(3)_f$ symmetry in the construction of ξ, whereas Ref. [7] neglects all $SU(3)_f$-breaking effects save for $\eta - \eta'$ mixing. In Ref. [7], ξ is replaced by the parameter e_0, namely

$$e_0 = \sqrt{\tfrac{2}{3}}\varepsilon + \sqrt{\tfrac{1}{3}}\varepsilon'. \tag{27}$$

Let us examine the ingredients of Eqs. (21) and (26). The ratios of $\bar{\Sigma}(M_1M_2)$ differ from unity if $SU(3)_f$ is broken in the light-cone distribution functions, through, specifically, the hard-spectator contributions to $\alpha_i(M_1M_2)$ [26]. The latter are real if the contribution of the twist-3 distribution amplitudes, which generate divergent, albeit formally power-suppressed, contributions, are neglected. This implies that the ratios of $\bar{\Sigma}(M_1M_2)$ in Eq. (21) are real, if all subleading corrections and electroweak penguin effects are neglected. The latter do make the ratios of $\bar{\Sigma}(M_1M_2)$ complex in leading order in $1/m_b$; however, electroweak penguin effects enter ξ in $\mathcal{O}(\alpha(m_d - m_u)/\Lambda_{\rm had})$, so that their inclusion is actually of higher order in isospin breaking. The remaining factors in Eq. (21) are given by

$$\left[\frac{A_{\eta_q^{(\prime)}\pi}}{A_{\pi\pi}}\right] = \frac{F_0^{B\to\eta^{(\prime)}}(0)}{F_0^{B\to\pi}(0)}, \tag{28}$$

where $F_0^{B\to M}$ denotes a form factor for the decay to a pseudoscalar meson M in the convention of Bauer, Stech, and Wirbel [28]. Following Beneke and Neubert, we parametrize [24]

$$F_0^{B\to\eta^{(\prime)}}(0) = F_1\frac{f^q_{\eta^{(\prime)}}}{f_\pi} + F_2\frac{\sqrt{2}f^q_{\eta^{(\prime)}} + f^s_{\eta^{(\prime)}}}{\sqrt{3}f_\pi}, \tag{29}$$

noting that $F_1/F_2 \sim \mathcal{O}(1)$ in the heavy-quark limit. The first term is related via $SU(3)_f$ breaking to $F_0^{B\to\pi}(0)$, where one expects $F_1 \approx F_0^{B\to\pi}(0)$ in the Feldmann-Kroll-Stech scheme [24]. The second term, however, is driven exclusively by the flavor-singlet contribution and cannot be related to $F_0^{B\to\pi}(0)$. It is ill-known, though likely of greater impact on the $B\to\eta'$ form factor [24].

1. Breaking the triangle relation

A nonzero value of the parameter ξ in Eq. (25) signals the breaking of the triangle relation, Eq. (6), and the appearance of an amplitude of $|\Delta I| = 5/2$ in character. In the QCD factorization approach, ξ is given by Eq. (26). If ξ can be determined with surety, and is real, an "isospin analysis" based on Eq. (25) can determine ϕ and $\bar{\phi}$ without theoretical error from this effect. Determining ξ requires the isospin-breaking parameters ε and ε', which characterize $\pi^0 - \eta, \eta'$ mixing, as well as $X_{\eta_q^{(\prime)}}$, as per Eq. (21). We begin by determining $X_{\eta_q^{(\prime)}}$ in the QCD factorization approach. The parameter $X_{\eta_q^{(\prime)}}$ is controlled by $F_0^{B\to\eta^{(\prime)}}/F_0^{B\to\pi}$ and $\Sigma(\eta_q\pi)/\Sigma(\pi\pi)$ exclusively, if power-suppressed contributions are indeed negligible. The former drives the numerical value of ξ. Using the parameters of Ref. [24], we find

$$\begin{aligned}\frac{F_0^{B\to\eta}(0)}{F_0^{B\to\pi}(0)} &= 0.83 \pm 0.02 \to 0.89\left[\sqrt{\frac{2}{3}} \approx 0.82\right],\\ \frac{F_0^{B\to\eta'}(0)}{F_0^{B\to\pi}(0)} &= 0.68 \pm 0.02 \to 1.1\left[\sqrt{\frac{1}{3}} \approx 0.58\right],\end{aligned} \tag{30}$$

where we emphasize that the uncertainties are dominated by that in F_2. To illustrate this, the first number in the reported range for each ratio employs $F_2 = 0$, whereas the second number employs, rather arbitrarily, $F_2 = 0.1$ as per Ref. [24]. The reported errors in the $F_2 = 0$ results are determined exclusively from the errors in the other inputs, assuming they are uncorrelated. For reference, we have also included, in brackets, the ratios assumed in the $SU(3)_f$ approach of Ref. [7]. The form factor ratio for the η' can differ substantially from that of Ref. [7], and varying the $\eta - \eta'$ mixing angle does not capture the excursion found. As for the remaining factor, we estimate, neglecting power corrections and electroweak penguin contributions,

$$\begin{aligned}\frac{\Sigma(\eta_q\pi)}{\Sigma(\pi\pi)} &\approx \frac{\alpha_1(\eta_q^{(\prime)}\pi) + \alpha_2(\eta_q^{(\prime)}\pi)}{\alpha_1(\pi\pi) + \alpha_2(\pi\pi)}\\ &\approx 1 + \frac{\alpha_s\pi f_{B_q}}{M_B\lambda_B}\frac{f_\pi}{F_0^{B\to\pi}}(1+\alpha_2^\pi)(\alpha_2^{\eta_q'} - \alpha_2^\pi)\\ &\approx 1 - 5\times 10^{-3},\end{aligned} \tag{31}$$

where the deviation from unity is determined by $SU(3)_f$ breaking in the light-cone distribution functions, as parametrized by α_2^M, which appear in the hard-spectator terms. We note, as in the case of annihilation contributions, that end-point divergences can appear in the power corrections. We employ the parameters given in Ref. [26] and observe that this source of $SU(3)_f$ breaking appears to be negligible. This observation is consistent with other recent data. For example, $SU(3)_f$ breaking in the form factors and decay constants suffices to explain the large difference in the observed branching ratios for $B_s \to K^+K^-$ and $B_d \to \pi^+\pi^-$ decays [29,30]. We thus determine

$$\begin{aligned}X_{\eta_q} &= 0.83 \pm 0.02 \to 0.89,\\ X_{\eta_q'} &= 0.68 \pm 0.02 \to 1.1,\end{aligned} \tag{32}$$

where the errors and ranges are determined precisely as discussed after Eq. (30). It is worth noting that the form of Eq. (24) is quite general; it does not rely on our adopted framework for $\eta - \eta'$ mixing. If, instead, a general, two-angle mixing formalism [31,32] in the octet-singlet basis were employed to describe $\eta - \eta'$ mixing, an equation of form Eq. (24) would nevertheless emerge [33]. We would also find compatible numerical results.[1] Indeed, we can use the empirical decay amplitudes to define and determine an effective parameter $\bar{X}^{\rm eff}_{\eta_q^{(\prime)}}$ via

$$A_{B^-\to\pi^-\eta^{(\prime)}} + \sqrt{2}A_{\bar{B}\to\pi^0\eta^{(\prime)}} = A_{B^-\to\pi^-\pi^0}\bar{X}^{\rm eff}_{\eta_q^{(\prime)}}, \tag{34}$$

where if power corrections, as well as isospin-breaking effects, are negligible, $\bar{X}^{\rm eff}_{\eta_q^{(\prime)}}$ is $\bar{X}_{\eta_q^{(\prime)}}$ as defined in Eq. (21). Empirical branching ratios for $B^-\to\pi^-\eta^{(\prime)}$, $\bar{B}\to\pi^0\eta^{(\prime)}$, and $B^-\to\pi^-\pi^0$ decays can thus eventually determine $|\bar{X}^{\rm eff}_{\eta_q^{(\prime)}}|$, and the angles $\mathrm{Arg}(A_{B^-\to\pi^-\eta^{(\prime)}}A^*_{B^-\to\pi^-\pi^0}\bar{X}^{\rm eff,*}_{\eta_q^{(\prime)}})$ and $\mathrm{Arg}(A_{\bar{B}\to\pi^0\eta^{(\prime)}}A^*_{B^-\to\pi^-\pi^0}\bar{X}^{\rm eff,*}_{\eta_q^{(\prime)}})$, up to discrete ambiguities. Data on the charge-conjugate modes would determine the charge conjugates of these quantities in a similar manner. Our theoretical analysis suggests that $\bar{X}^{\rm eff}_{\eta_q^{(\prime)}}$ is real to a good approximation,[2] so that the deduced empirical angles can be interpreted as $\mathrm{Arg}(A_{B^-\to\pi^-\eta^{(\prime)}}A^*_{B^-\to\pi^-\pi^0})$ and $\mathrm{Arg}(A_{\bar{B}\to\pi^0\eta^{(\prime)}}A^*_{B^-\to\pi^-\pi^0})$ [7]. Nevertheless, verifying that $|\bar{X}^{\rm eff}_{\eta_q^{(\prime)}}| = |X^{\rm eff}_{\eta_q^{(\prime)}}|$, e.g., would serve as a consistency check. We thus expect that this analysis would not only constrain the ill-known $B\to\eta^{(\prime)}$ form factors, but also help determine the extent to which $\Delta\alpha_{\rm isospin}\neq\Delta\alpha$, as we shall explain.

Before turning to this issue, let us conclude by determining the expected value of the $|\Delta I| = 5/2$ parameter ξ and the manner in which its uncertainty impacts $\Delta\alpha_{\rm isospin}$. To compute ξ, we use the recent results of Kroll for the $\pi^0-\eta,\eta'$ mixing angles [34]:

$$\varepsilon = 0.017\pm 0.003; \qquad \varepsilon' = 0.004\pm 0.001, \tag{35}$$

to yield

$$\xi = 0.017\pm 0.003 \to 0.020 \quad [0.016], \tag{36}$$

where the error in ξ is determined from those of the inputs alone, assuming their errors are uncorrelated. We have incorporated the $\pi^0-\eta,\eta'$ mixing angles directly as determined in low-energy experiments; we note that the scale dependence of the light-cone distribution functions, of which this is part, does not enter at next-to-leading order accuracy in α_s [23]. The results employ F_2 as in Eq. (30) and report, in brackets, the value found in the $\mathrm{SU}(3)_f$ analysis of Ref. [7] as well. Note that the greater uncertainty in $X_{\eta'_q}$ noted previously has little bearing on the final error in ξ, as the $\pi^0-\eta'$ mixing angle ε' is relatively small. Given an estimate of ξ and its error, we can also proceed to determine the uncertainty in ϕ consequent to it. To do this, we note that $\cos\phi$ can be determined from the empirical decay amplitudes, determined from the empirical branching ratios via Eqs. (4) and (5), and the relationship given in Eq. (25).[3] We employ Eq. (3) for the neutral modes, but define in this case

$$|A_2| = \tfrac{2}{3}(1-\xi)|A_{B^+\to\pi^+\pi^0}|, \tag{37}$$

to yield

$$\cos\phi = \cos\phi_0 + \xi\left(\cos\phi_0 - \sqrt{2}\frac{|A_{B^+\to\pi^+\pi^0}|}{|A_{B\to\pi^+\pi^-}|}\right) + \mathcal{O}(\xi^2), \tag{38}$$

where

$$\cos\phi_0 = \frac{1}{2\sqrt{2}} \times\left[\frac{|A_{B\to\pi^+\pi^-}|^2 - |A_{B\to\pi^0\pi^0}|^2 + 2|A_{B^+\to\pi^+\pi^0}|^2}{|A_{B^+\to\pi^+\pi^0}||A_{B\to\pi^+\pi^-}|}\right]. \tag{39}$$

The error in ξ generates an error in the determination of ϕ; namely, $\sigma_\phi = \sigma_\xi|\partial\phi/\partial\xi|$, where we note that the error in $\bar{\phi}$ follows from replacing the amplitudes by their CP conjugates. Assuming a 100% error in our estimate of σ_ξ, as F_2 is ill-known and the $\pi^0-\eta,\eta'$ mixing angles can have a small electromagnetic component, estimated to be some 6% of ε_8 [20], we employ $\sigma_\xi = 0.006$ and a recent empirical compilation of CP-averaged branching ratios [12], reported in Table I, to estimate $\sigma_\phi = 0.4°$ and thus an error in $\Delta\alpha_{\rm isospin}$ of 0.4°, as we add the errors linearly. In contrast, the shift in ϕ due to the $\mathcal{O}(\xi)$ contribution is 1.2°. We note, in particular, that our error estimate can be made more robust, if not reduced, through the measurement of $B\to\pi\eta^{(\prime)}$ decays.

2. Breaking $\Delta\alpha_{\rm isospin} = \Delta\alpha$

Thus far we have determined the error in $\Delta\alpha_{\rm isospin}$ incurred through the uncertainty in the parameter ξ. The error in $\Delta\alpha$, however, is determined by that in

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[1] In a two-angle mixing formalism, assuming as per Ref. [24], that the ratios of the $B\to\eta^{(\prime)}$ and $B\to\pi$ form factors are determined by the ratios of the related decay constants, we have

$$\frac{F_0^{B\to\eta}(0)}{F_0^{B\to\pi}(0)} = \frac{\sqrt{2}}{f_\pi}\left(\frac{f_8\cos\theta_8}{\sqrt{6}} - \frac{f_0\sin\theta_0}{\sqrt{3}}\right),$$
$$\frac{F_0^{B\to\eta'}(0)}{F_0^{B\to\pi}(0)} = \frac{\sqrt{2}}{f_\pi}\left(\frac{f_8\sin\theta_8}{\sqrt{6}} + \frac{f_0\cos\theta_0}{\sqrt{3}}\right). \tag{33}$$

If $f_8 = f_0 = f_\pi$ and $\theta_8=\theta_0=\theta$ and we assume the ideal mixing angle $\theta = \sin^{-1}(-1/3)$ we recover $F_0^{B\to\eta}(0)/F_0^{B\to\pi}(0) = \sqrt{2/3}$ and $F_0^{B\to\eta'}(0)/F_0^{B\to\pi}(0) = \sqrt{1/3}$ as per Ref. [7]. If we employ the parameters in either Eq. (3.7) or Eq. (3.8) of Ref. [32] we find results comparable to what we have reported in the $F_2 = 0$ case.

[2] The $\mathrm{SU}(3)_f$-breaking electroweak penguin contribution to $\Sigma(\eta_q^{(\prime)})/\Sigma(\pi\pi)$ generates the only complex contribution in leading power in $1/m_b$. Note that of the neglected annihilation terms, only the electroweak penguin annihilation contributions can be complex.

[3] The sign of ϕ is undetermined.

TABLE I. CP-averaged branching ratios for selected $B \to PP$ modes from the compilation of Ref. [12], reported as $10^6\,\mathrm{Br}(B \to PP)$. We display the experimental data, both preliminary and published, available since the compilation of Ref. [35] and included in the averages of Ref. [12].

Mode PP	PDG [35]	*BABAR*	Belle	CLEO	CDF [36]	HFAG [12]
$\pi^+\pi^0$	$5.6^{+0.9}_{-1.1}$	$5.8 \pm 0.6 \pm 0.4$ [37]	$5.0 \pm 1.2 \pm 0.5$ [38]	$4.6^{+1.8+0.6}_{-1.6-0.7}$ [39]		5.5 ± 0.6
$\eta\pi^+$	<5.7	$5.1 \pm 0.6 \pm 0.3$ [40]	$4.8 \pm 0.7 \pm 0.3$ [41]	$1.2^{+2.8}_{-1.2}$ [42]		4.9 ± 0.5
$\eta'\pi^+$	<7	$4.0 \pm 0.8 \pm 0.4$ [40]	<7 [43]	$1.0^{+5.8}_{-1.0}$ [42]		4.0 ± 0.9
$\pi^+\pi^-$	4.8 ± 0.5	$4.7 \pm 0.6 \pm 0.2$ [44]	$4.4 \pm 0.6 \pm 0.3$ [38]	$4.5^{+1.4+0.5}_{-1.2-0.4}$ [39]	4.4 ± 1.3	4.5 ± 0.4
$\pi^0\pi^0$	1.9 ± 0.5	$1.17 \pm 0.32 \pm 0.10$ [37]	$2.3^{+0.4+0.2}_{-0.5-0.3}$ [45]	<4.4 [39]		1.45 ± 0.29
$\eta\pi^0$	<2.9	<2.5 [46]	<2.5 [41]	<2.9 [42]		<2.5
$\eta'\pi^0$	<5.7	<3.7 [46]		<5.7 [42]		<3.7

$$\Delta\alpha = \Delta\alpha_{\mathrm{isospin}} + \tfrac{1}{2}\mathrm{Arg}(e^{2i\gamma}\bar{A}_{-0}A^*_{+0}). \tag{40}$$

Defining $\zeta \equiv \mathrm{Arg}(A_{B^+\to\pi^+\pi^0}T^*)$ and $\bar{\zeta} \equiv \mathrm{Arg}(\bar{A}_{B^-\to\pi^-\pi^0}\bar{T}^*)$, where T is the tree-level contribution to $B^+ \to \pi^+\pi^0$ decay in the isospin-perfect limit, so that $|T| = |\bar{T}|$, we have

$$\mathrm{Arg}\,(e^{2i\gamma}\bar{A}_{-0}A^*_{+0}) = \bar{\zeta} - \zeta. \tag{41}$$

The interplay of these relationships is illustrated in Fig. 1. As in the isospin-perfect case, the angle ϕ has a discrete ambiguity, as does the angle ζ: their overall sign is not determined. This is realized as an ambiguity in the orientation of $\triangle ABC$, that is, whether it points up or down. A similar ambiguity also exists for the charge-conjugate amplitudes, which yield $\bar{\phi}$ and $\bar{\zeta}$, to yield a four-fold ambiguity in $\Delta\alpha$. The angles ζ and $\bar{\zeta}$ are nonzero if penguin contributions of $|\Delta I| = 3/2$ character occur. We wish to estimate the extent to which $\Delta\alpha \neq \Delta\alpha_{\mathrm{isospin}}$, as well as its uncertainty, though we shall begin by considering the contribution from $\pi^0 - \eta, \eta'$ mixing exclusively.

In the presence of $\pi^0 - \eta, \eta'$ mixing, we have

$$A_{B^+\to\pi^+\pi^0} = A_{B^+\to\pi^+\phi_3} + \varepsilon A_{B^+\to\pi^+\eta} + \varepsilon' A_{B^+\to\pi^+\eta'}, \tag{42}$$

with $A_{B^+\to\pi^+\phi_3} = T + P_{\mathrm{ew}}$, where we emphasize that the

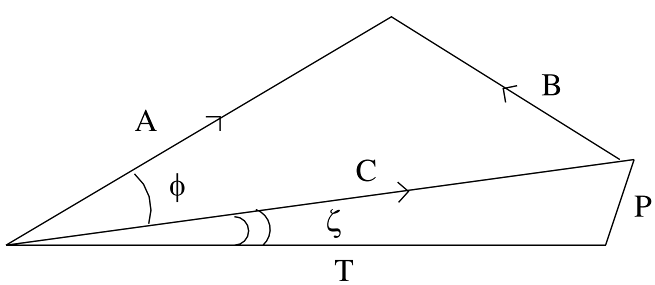

FIG. 1. Schematic illustration of the triangle relation in $B \to \pi\pi$ decay in the presence of isospin breaking, Eq. (25). Note that $A \equiv A_{B\to\pi^+\pi^-}/\sqrt{2}$, $B \equiv A_{B\to\pi^0\pi^0}/\sqrt{2}$, and $C \equiv (1-\xi)A_{B^+\to\pi^+\pi^0}$. Moreover, ξ is real, with $A_{B^+\to\pi^+\pi^0} = T + P$, where T is the tree-level contribution to $B^+ \to \pi^+\pi^0$ decay in the isospin-perfect limit.

amplitude computed with the $I = 1$, $I_3 = 0$ state ϕ_3 can contain an $|\Delta I| = 3/2$ electroweak penguin contribution, P_{ew}, in addition to a tree-level contribution T. The angle ζ can be written as

$$\zeta = \mathrm{Arg}(A_{B^+\to\pi^+\pi^0}A^*_{B^+\to\pi^+\phi_3}) + \mathrm{Arg}(A_{B^+\to\pi^+\phi_3}T^*), \tag{43}$$

where the first term is of $\mathcal{O}(\varepsilon, \varepsilon')$ and the second is rendered nonzero by P_{ew}. Here we focus on the first term, namely,

$$\begin{aligned}\zeta_{\eta,\eta'} &\equiv \mathrm{Arg}(A_{B^+\to\pi^+\pi^0}A^*_{B^+\to\pi^+\phi_3}) \\ &= \varepsilon\sin\theta_\eta\frac{|A_{B^+\to\pi^+\eta}|}{|A_{B^+\to\pi^+\pi^0}|} + \varepsilon'\sin\theta_{\eta'}\frac{|A_{B^+\to\pi^+\eta'}|}{|A_{B^+\to\pi^+\pi^0}|} \\ &= \varepsilon\sin\theta_\eta\sqrt{\frac{\gamma(B^+\to\pi^+\eta)}{\gamma(B^+\to\pi^+\pi^0)}} \\ &\quad + \varepsilon'\sin\theta_{\eta'}\sqrt{\frac{\gamma(B^+\to\pi^+\eta')}{\gamma(B^+\to\pi^+\pi^0)}},\end{aligned} \tag{44}$$

where we work in $\mathcal{O}(\varepsilon, \varepsilon')$ throughout, with

$$\theta_{\eta^{(\prime)}} \equiv \mathrm{Arg}(A_{B^+\to\pi^+\eta^{(\prime)}}A^*_{B^+\to\pi^+\pi^0}). \tag{45}$$

Defining analogous variables for the CP-conjugate amplitudes, we determine that the contribution to $\Delta\alpha - \Delta\alpha_{\mathrm{isospin}}$ from $\pi^0 - \eta, \eta'$ mixing is

$$\begin{aligned}\frac{1}{2}(\bar{\zeta}_{\eta,\eta'} - \zeta_{\eta,\eta'}) = \frac{\varepsilon}{2}\Bigg(&\sin\bar{\theta}_\eta\sqrt{\frac{\gamma(B^-\to\pi^-\eta)}{\gamma(B^-\to\pi^-\pi^0)}} \\ &- \sin\theta_\eta\sqrt{\frac{\gamma(B^+\to\pi^+\eta)}{\gamma(B^+\to\pi^+\pi^0)}}\Bigg) \\ + \frac{\varepsilon'}{2}\Bigg(&\sin\bar{\theta}_{\eta'}\sqrt{\frac{\gamma(B^-\to\pi^-\eta')}{\gamma(B^-\to\pi^-\pi^0)}} \\ &- \sin\theta_{\eta'}\sqrt{\frac{\gamma(B^+\to\pi^+\eta')}{\gamma(B^+\to\pi^+\pi^0)}}\Bigg).\end{aligned} \tag{46}$$

Letting $\sin\bar{\theta}_{\eta^{(\prime)}} = -\sin\theta_{\eta^{(\prime)}} = 1$ and employing the empirical, CP-averaged branching ratios of the compilation of Ref. [12], we estimate

$$\tfrac{1}{2}(\bar{\zeta}_{\eta,\eta'} - \zeta_{\eta,\eta'}) \lesssim 1.3^\circ, \tag{47}$$

at 67% confidence interval. An implicit error, of 0.2°, follows from the errors in the branching ratios and $\pi^0 - \eta, \eta'$ mixing angles alone, assuming such are uncorrelated. Note that we have added the errors in $\bar{\zeta}_{\eta,\eta'}$ and $\zeta_{\eta,\eta'}$ linearly. This numerical result can be compared to the bound of 1.6° at 90% confidence level reported in Ref. [7]; our bound is slightly smaller as it employs measured branching ratios, rather than experimental bounds. Its provenance is also different, as the bound in our case does not depend on an assertion of $\mathrm{SU}(3)_f$ symmetry. Most importantly, it is improvable, as it is driven by empirical errors. In addition, the angles $\bar{\theta}_{\eta^{(\prime)}}$ and $\theta_{\eta^{(\prime)}}$ are also subject to empirical constraint, so that a direct assessment of $(\bar{\zeta}_{\eta,\eta'} - \zeta_{\eta,\eta'})/2$ should eventually prove possible. Ultimately, it is the uncertainty in $(\bar{\zeta}_{\eta,\eta'} - \zeta_{\eta,\eta'})/2$ which matters, not its gross deviation from zero.

B. Other isospin-breaking effects

Thus far we have considered the disparate roles of $\pi^0 - \eta, \eta'$ mixing: this isospin-breaking effect can not only engender a $|\Delta I| = 5/2$ amplitude, breaking the triangle relation of Eq. (6), but also generate a $|\Delta I| = 3/2$ penguin amplitude, forcing $\Delta\alpha_{\mathrm{isospin}} - \Delta\alpha \neq 0$. Yet isospin breaking is not limited to $\pi^0 - \eta, \eta'$ mixing, and we can ask what other effects might enter, as well as how we might discern their presence from the experimental data.

As we have mentioned, $|\Delta I| = 3/2$ electroweak penguin contributions can contribute to $\Delta\alpha_{\mathrm{isospin}} - \Delta\alpha \neq 0$, through the second term of Eq. (43). If one neglects the electroweak penguin operators associated with small Wilson coefficients, namely c_7 and c_8 [11], then the impact of these contributions on $\Delta\alpha$ can be assessed, without theoretical ambiguity, up to isospin-violating corrections [5], to yield [7]

$$(\Delta\alpha - \Delta\alpha_{\mathrm{isospin}})_{\mathrm{ewp}} = 1.5^\circ \pm 0.3^\circ, \tag{48}$$

where the error arises from that in the empirical inputs. Isospin breaking in the matrix elements of the strong-penguin operators can also engender a $|\Delta I| = 3/2$ contribution [6,14], not captured by $\pi^0 - \eta, \eta'$ mixing. For example, corrections of $\mathcal{O}(\alpha)$ can distinguish $A_{\pi^\pm\phi_3}$ from $A_{\phi_3\pi^\pm}$, or, specifically, $F_0^{B^\pm\to\pi^\pm}(0)f_{\phi_3}$ from $F_0^{B^\pm\to\phi_3}(0)f_{\pi^\pm}$. In addition, $m_d \neq m_u$ effects beyond $\pi^0 - \eta, \eta'$ mixing can also occur [14,15], though in $K \to \pi\pi$ decay, e.g., such terms do not appear in the weak chiral Lagrangian in $\mathcal{O}(p^2)$ [47]. The contributions from electroweak penguin operators should yield the largest effect [6]. In particular, we note, using the notation of Ref. [23], that $\alpha|C_4|/|C_9| \sim 4\%$.

Contributions to the $|\Delta I| = 5/2$ amplitude, not mediated by $\pi^0 - \eta, \eta'$ mixing, can also occur. For example, $\mathcal{O}(\alpha)$ effects in the evaluation of $F_0^{B\to\pi}$ and f_π can yield an effective $|\Delta I| = 5/2$ amplitude from either $|\Delta I| = 3/2$ or $|\Delta I| = 1/2$ weak transition operators. Contributions built on the former can be absorbed by modifying ξ and $\bar{\xi}$ and enlarging their errors. Contributions built on the latter are more problematic, as they will make ξ and $\bar{\xi}$ complex, as well as $\xi \neq \bar{\xi}$. Consequently, the angle determined from the analysis of Eq. (25), i.e., $\phi' \equiv \mathrm{Arg}(A_{+-}(1 - \xi^*)A^*_{B^+\to\pi^+\pi^0})$, is not ϕ. A similar conclusion emerges from the study of the charge-conjugate amplitudes, where we note $\bar{\phi}' \equiv \mathrm{Arg}(\bar{A}_{+-}(1 - \bar{\xi}^*)A^*_{B^+\to\pi^+\pi^0})$ is not $\bar{\phi}$. Generally we can rewrite Eq. (40) as

$$\Delta\alpha = \tfrac{1}{2}(\bar{\phi}' - \phi') + \tfrac{1}{2}(\bar{\zeta} - \zeta) + \tfrac{1}{2}[(\bar{\phi} - \phi) - (\bar{\phi}' - \phi')], \tag{49}$$

where the last term vanishes if ξ and $\bar{\xi}$ are real. Note that the geometric interpretation of ϕ and ζ illustrated in Fig. 1, as well as of $\bar{\phi}$ and $\bar{\zeta}$, make the signed contributions of $(\bar{\phi} - \phi)/2$ and $(\bar{\zeta} - \zeta)/2$, and, by inference, $(\bar{\phi}' - \phi')/2$ and $(\bar{\zeta} - \zeta)/2$, add constructively. The sign of the term $[(\bar{\phi} - \phi) - (\bar{\phi}' - \phi')]/2$, however, is unclear. Nevertheless, in contradistinction to $K \to \pi\pi$ decays [8,48,49], we do expect the role of the $|\Delta I| = 1/2$ weak transition in generating an effective $|\Delta I| = 5/2$ amplitude in $B \to \pi\pi$ decays to be a relatively small effect. That is, on general grounds, the pattern of empirical branching ratios shows that the $|\Delta I| = 1/2$ amplitude is not dominant, indeed that $|A_{3/2,2}| \gtrsim |A_{1/2,2}|$, and $\alpha/\varepsilon \approx 0.4$. It is worth noting, though, that ξ and $\bar{\xi}$ can be complex from the inclusion of $\pi^0 - \eta, \eta'$ effects alone. However, such effects arise, in leading power, from $\mathrm{SU}(3)_f$ breaking in the light-cone distributions functions of the $\eta^{(\prime)}$ and π which appear in the electroweak penguin contributions and, in the power corrections, through the electroweak penguin annihilation contributions. We find the leading-power effect to be negligibly small, though testing, as per Eq. (34), whether $|X^{\mathrm{eff}}_{\eta_q^{(\prime)}}| = |\bar{X}^{\mathrm{eff}}_{\eta_q^{(\prime)}}|$ is borne out by experiment should reveal the presence of unexpectedly large complex contributions.

IV. SUMMARY

The study of $B \to \pi\pi$ decays under an assumption of isospin symmetry permits the extraction of the angle α, modulo discrete ambiguities. This is realized through the determination of the penguin pollution $\Delta\alpha$, which is also discretely ambiguous, yielding $\alpha = \alpha_{\mathrm{eff}} - \Delta\alpha$ from the directly measured quantity $\sin(2\alpha_{\mathrm{eff}})$. Isospin symmetry is broken in nature, as the up and down quarks differ in both their mass and charge, and it is important to assess the error thus incurred on $\Delta\alpha$. We have studied isospin-breaking effects in $B \to \pi\pi$ decays, placing particular emphasis on the role of $\pi^0 - \eta, \eta'$ mixing, as it yields the most significant effects. In particular, $\pi^0 - \eta, \eta'$ mixing can not only engender a $|\Delta I| = 5/2$ amplitude, breaking the triangle relation of Eq. (6), but also generate a $|\Delta I| = 3/2$ penguin amplitude, forcing $\Delta\alpha_{\rm isospin} - \Delta\alpha \neq 0$.

We recognize that, in nature, all flavor symmetries are approximate, and we have computed the shift in $\Delta\alpha$ to leading order in isospin breaking, with an assessment of the error in this shift. To realize this, we have worked within the QCD factorization framework, though our results do not depend on the details of such an analysis. Rather, the essential point is the utility of a combined heavy-quark, $1/m_b$, and α_s expansion of the theoretical decay amplitudes. We use it to sort through the various effects, to determine that the empirical $B \to \pi\pi$ amplitudes satisfy a modified triangle relation, Eq. (25), with an isospin-breaking parameter ξ which is real, to good approximation. Moreover, under the assumption that ξ is real and determined exclusively by $\pi^0 - \eta, \eta'$ mixing, its value can be determined from experiment, once information on the $\pi^0 - \eta, \eta'$ mixing angles is employed. Indeed, the essential improvements over the analysis of Ref. [6] are these: that a relationship of form Eq. (25) exists with a real parameter ξ and that empirical information on $B \to \pi\eta^{(\prime)}$ decays exists and can be employed to constrain the impact of isospin-breaking effects. This is important, as the $B \to \eta^{(\prime)}$ form factors contain contributions which are not constrained by $SU(3)_f$ symmetry [24]. The empirical data on $B \to \pi\eta^{(\prime)}$ decays is incomplete, though it can be expected to improve. Nevertheless, enough information currently exists to realize a crucial shift in our perception of isospin-breaking effects. What matters is not the shift in $\Delta\alpha$ *per se*, but rather the surety with which we can assess that shift. We assess that the change in $\Delta\alpha$ due to isospin-breaking effects, namely $\delta(\Delta\alpha) \equiv \Delta\alpha - \Delta\alpha_0$, where $\Delta\alpha_0$ represents the penguin pollution in the isospin-perfect limit, is

$$\delta(\Delta\alpha) = 1.2^\circ[\xi] + 1.5^\circ[P_{\rm ew}] + 1.3^\circ[P_{\pi^0-\eta,\eta'}, \text{bound}] + \ldots \approx 4^\circ, \tag{50}$$

where we have resolved the discrete ambiguity in $\Delta\alpha$ by assuming that $\bar{\phi} > 0$ and $\phi < 0$. We note, currently, that $\alpha = (101^{+16}_{-9})^\circ$ [12,50]; no corrections from isospin-breaking effects have been included. The contribution labeled "ξ" is the shift in $\Delta\alpha$ due to the presence of a $A_{5/2,2}$ amplitude, realized through $\pi^0 - \eta, \eta'$ mixing only. This is neglected in the numerical estimates of Ref. [7]. The contributions labeled "$P_{\rm ew}$" and "$P_{\pi^0-\eta,\eta'}$" represent the shift in $\Delta\alpha$ due to penguin contributions of effective $|\Delta I| = 3/2$ character. We emphasize that the latter number is a bound, rather than an explicit estimate. The ellipsis includes neglected isospin-breaking contributions, such as $A_{5/2,2}$ contributions generated by $\mathcal{O}(\alpha)$ effects on the $|\Delta I| = 1/2$ weak transition, which should be rather smaller than the estimate labeled by ξ. However, the errors in these estimates are smaller and are insensitive to the manner in which the discrete ambiguity in $\Delta\alpha$ is resolved:

$$\sigma_\alpha^{\rm IB} = 0.4^\circ[\xi] + 0.3^\circ[P_{\rm ew}] + 1.3^\circ[P_{\pi^0-\eta,\eta'}, \text{bound}] + \ldots \approx 2^\circ, \tag{51}$$

and it is improvable. Note, in particular, the error associated with the $A_{5/2,2}$ amplitude comes from doubling the error in the theoretical computation of ξ; here we employ the theoretical range in the $F_0^{B\to\eta^{(\prime)}}$ form factors recommended by Ref. [24]. This error can be tested, if not mitigated, through the use of anticipated empirical data. Note, too, that we have included the bound from penguin contributions to $B^\pm \to \pi^\pm\pi^0$ decays from $\pi^0 - \eta, \eta'$ mixing in our theory error. This can be mitigated with improved empirical data. Ultimately, we believe that a theoretical systematic error $\sigma_\alpha^{\rm IB}$ of $\mathcal{O}(1^\circ)$ is attainable.

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