How Isospin Violation Mocks “New” Physics: 
$\pi^0$-$\eta, \eta'$ Mixing in $B \to \pi\pi$ Decays

S. Gardner
Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506-0055 USA
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Abstract

An isospin analysis of $B \to \pi\pi$ decays yields $\sin 2\alpha$, where $\alpha \equiv \arg[-V_{td}V_{tb}^*/(V_{ud}V_{ub}^*)]$ and $V_{ij}$ is a CKM matrix element, without hadronic uncertainty if isospin is a perfect symmetry. Isospin, however, is broken not only by electroweak effects but also by the $u$ and $d$ quark mass difference. The latter drives $\pi^0 - \eta, \eta'$ mixing and converts the isospin-perfect triangle relation between the $B \to \pi\pi$ amplitudes to a quadrilateral. The combined isospin-violating effects impact the extracted value of $\sin 2\alpha$ in a significant manner, particularly if the latter is small.

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In the standard model, CP violation is characterized by a single phase in the Cabibbo-Kobayashi-Maskawa (CKM) matrix, rendering its elements complex. Although CP violation has been known in the neutral kaon system since 1964, the absence of definitive evidence for a non-zero $\varepsilon'$ parameter leaves the above standard model picture unsubstantiated [1]. Indeed, probing the precise mechanism of CP violation will be the primary mission of the future B factories. The CKM matrix of the standard model is unitary, so that determining whether or not this is empirically so results in a non-trivial test of the standard model’s veracity. In the CKM matrix, only one combination of rows and columns results in an unitarity test in which all the terms are of the same approximate magnitude [2]; this is the unitarity triangle [3]. Empirically determining whether its angles, termed $\alpha$, $\beta$, and $\gamma$, sum to $\pi$ and whether its angles are compatible with the measured lengths of its sides lie at the heart of these tests of the standard model.

In the decay of a neutral $B$ meson to a CP eigenstate $f_{CP}$, CP violation can be generated through $B^0-\overline{B}^0$ mixing, specifically through the interference of $B^0 \to f_{CP}$ and $B^0 \to \overline{B}^0 \to f_{CP}$. Thus, weak phase information can be extracted from the time-dependent asymmetry $A(t)$, defined as

$$A(t) = \frac{\Gamma(B^0(t) \to f_{CP}) - \Gamma(\overline{B}^0(t) \to f_{CP})}{\Gamma(B^0(t) \to f_{CP}) + \Gamma(\overline{B}^0(t) \to f_{CP})},$$

noting $B^0(t = 0) = B^0$ and $\overline{B}^0(t = 0) = \overline{B}^0$. Indeed, were only amplitudes with a single CKM phase to contribute to $B^0(t = 0) \to f_{CP}$, the weak phase information could be extracted directly from $A(t)$ without hadronic ambiguity [3]. Unfortunately, however, either penguin contributions or a plurality of tree-level contributions arise to cloud the above analysis [4].

Nevertheless, the quantity $\sin 2\alpha$, where $\alpha$ is the usual CKM angle $\alpha \equiv \arg[-V_{ud}V_{ub}^*/(V_{ud}V_{ub}^*)]$ [3], can be extracted without penguin “pollution” from an isospin analysis of $B \to \pi\pi$ decays if isospin is a perfect symmetry [3]. In this limit, the Bose symmetry of the $J = 0$ $\pi\pi$ state permits amplitudes merely of isospin $I = 0, 2$. This implies that the amplitude $B^\pm \to \pi^\pm \pi^0$ is purely $I = 2$. Thus, as two independent amplitudes describe the three amplitudes $B^+ \to \pi^+ \pi^0$, $B^0 \to \pi^+ \pi^-$, and $B^0 \to \pi^0 \pi^0$, they can be drawn as a triangle. A triangle can also be formed from the amplitudes $B^- \to \pi^- \pi^0$, $\overline{B}^0 \to \pi^+ \pi^-$, and $\overline{B}^0 \to \pi^0 \pi^0$, with the $B^\pm \to \pi^\pm \pi^0$ amplitudes forming a common base. The strong penguin contributions are of $\Delta I = 1/2$ character, so that they cannot contribute to the $I = 2$ amplitude and no CP violation is possible in the $\pi^\pm \pi^0$ final states. This implies that the CP violation due to the penguin contribution in $B^0 \to \pi^+ \pi^-$, or analogously in $\overline{B}^0 \to \pi^+ \pi^-$, can be isolated and removed by identifying the relative magnitude and phase of the $I = 0$ and $I = 2$ amplitudes.

It is our purpose to examine the manner in which isospin-violating effects impact the extraction of $\sin 2\alpha$ as determined in $B \to \pi\pi$ decays [4]. In the standard model, isospin is an approximate symmetry. Isospin is broken not only by electroweak effects but also by the strong interaction through the $u$ and $d$ quark mass difference. Both sources of isospin violation generate $\Delta I = 3/2$ penguin contributions, but the latter also drives $\pi^0 - \eta, \eta'$ mixing [3], admitting an $I = 1$ amplitude [3]. These latter contributions convert the triangle relations between the amplitudes to quadrilaterals. The effect of electroweak penguins has
been studied earlier in the literature, and is estimated to be small \[4,8,9\]. Nevertheless, when all the effects of isospin violation are included, the impact on the extracted value of \(\sin 2\alpha\) is significant.

To review the isospin analysis in \(B \to \pi \pi\) decays \[1\], let us consider the time-dependent asymmetry \(A(t)\) \[3\]:

\[
A(t) = \frac{(1 - |r_{f_{\text{CP}}}|^2)}{(1 + |r_{f_{\text{CP}}}|^2)} \cos(\Delta m t) - \frac{2(\text{Im}\, r_{f_{\text{CP}}})}{(1 + |r_{f_{\text{CP}}}|^2)} \sin(\Delta m t),
\]

where \(r_{f_{\text{CP}}} = (V_{ub}V_{ud}^*/V_{tb}V_{td}^*) \frac{A^{f_{\text{CP}}}/A^{CP}}{A^{f_{\text{CP}}} = A(B_0^0 \to f_{\text{CP}})}\). We assume the mass eigenstates \(B_L\) and \(B_H\) have the same width and a mass difference \(\Delta m \equiv B_H - B_L\). The \(\sin(\Delta m t)\) term, resulting from \(B^0-B^0\) mixing, is linear in \(r_{f_{\text{CP}}}\) and thus is of especial interest. If \(f_{\text{CP}} = \pi \pi\), then the presence of penguin contributions implies \(A^{f_{\text{CP}}} \neq A^{\text{CP}}\). We denote the amplitudes \(B^+ \to \pi^+\pi^0\), \(B^0 \to \pi^0\pi^0\), and \(B^0 \to \pi^+\pi^−\), by \(A^+, A^{00}, \text{and } A^{+−}\), respectively, and, following Ref. \[3\], we write

\[
\frac{1}{2} A^{+−} = A_2 - A_0; \quad A^{00} = 2A_2 + A_0; \quad \frac{1}{\sqrt{2}} A^{+0} = 3A_2,
\]

noting analogous relations for \(A^{−0}, \overline{A}^{00}, \text{and } \overline{A}^{+−}\) in terms of \(A_2\) and \(A_0\). Thus,

\[
|A_\pi^+\pi^-| = e^{-2i\phi_m} \frac{(A_2 - A_0)}{(A_2 - A_0)} = e^{2i\alpha (1 - 2z)},
\]

where \(z(\overline{z}) \equiv A_0/A_2(A_0/A_2)\) and \(A_2/A_2 = \exp(−2i\phi_t)\) with \(\phi_t \equiv \arg(V_{ud}V_{ub}^*)\) and \(\phi_m + \phi_t = \beta + \gamma = \pi - \alpha\) in the standard model \[3\]. Given \(|A^{+−}|, |A^{00}|, |A^{+0}|\), and their charge conjugates, the measurement of \(\text{Im}\, r_{\pi^+\pi^-}\) determines \(\sin 2\alpha\), modulo discrete ambiguities in \(\arg((1-\overline{z})/(1-z))\). The latter can be removed via a measurement of \(\text{Im}\, r_{\pi^0\pi^0}\) as well \[3\].

We proceed by computing the individual amplitudes using the \(\Delta B = 1\) effective Hamiltonian resulting from the operator product expansion in QCD in next-to-leading logarithmic (NLL) order \[10,11\], using the factorization approximation for the hadronic matrix elements. The factorization approximation, which assumes the four-quark-operator matrix elements to be saturated by vacuum intermediate states, finds theoretical justification in the large \(N_c\) limit of QCD \[11\] and phenomenological justification in comparison with empirical branching ratios \[12\]; nevertheless, it is heuristic. We adopt it in order to construct concrete estimates of the effects of isospin violation in the decays of interest. In this context, we can then apply the isospin analysis delineated above to infer \(\sin 2\alpha\) and thus estimate its theoretical systematic error, incurred through the neglect of isospin violating effects.

The effective Hamiltonian \(\mathcal{H}^{\text{eff}}\) for \(b \to d\bar{q}q\) can be parametrized as \[11\]

\[
\mathcal{H}^{\text{eff}} = \frac{G_F}{\sqrt{2}} \left[ V_{ub}V_{ud}^*(C_1 O_1^u + C_2 O_2^u) + V_{cb}V_{cd}^*(C_1 O_1^c + C_2 O_2^c) - V_{tb}V_{td}^* \left( \sum_{i=3}^{10} C_i O_i + C_9 O_9 \right) \right],
\]

where \(O_i\) and \(O_j\) are as per Ref. \[11\]; we also adopt their Wilson coefficients \(C_i\) and \(C_j\), computed in the naive dimensional regularization scheme at a renormalization scale of \(\mu = 2.5\)
are complex and depend on both the CKM matrix parameters and $\chi_m q$.

The transition form factors are given by

$$\langle dq\bar{q} | \mathcal{H}_{\text{eff}} | b \rangle = (G_F / \sqrt{2}) \langle dq\bar{q} | [V_{ub} V_{td} (C_{1}^{\text{eff}} O_{1}^{\pi} + C_{2}^{\text{eff}} O_{2}^{\pi}) - V_{tb} V_{td} \sum_{i=3}^{10} C_{i}^{\text{eff}} O_{i}^{\pi}] | b \rangle_{\text{tree}},$$

where “tree” denotes a tree-level matrix element and the $C_{i}^{\text{eff}}$ are from Ref. [10]. The $C_{i}^{\text{eff}}$ are complex and depend on both the CKM matrix parameters and $k^2$, where $k$ is the momentum transferred to the $q\bar{q}$ pair in $b \to dq\bar{q}$. Noting Ref. [2] we use $\rho = 0.12$, $\eta = 0.34$, and $\lambda = 0.2205$ unless otherwise stated. One expects $m_b^2 / 4 \lesssim k^2 \lesssim m_b^2 / 2$; we use $k^2 / m_b^2 = 0.3, 0.5$ in what follows.

To include the effects of $\pi^0 - \eta, \eta'$ mixing, we write the pion mass eigenstate $|\pi^0\rangle$ in terms of the $SU(3)_f$ perfect states $|\phi_0\rangle = |u\bar{u} - d\bar{d}|/\sqrt{2}$, $|\phi_8\rangle = |u\bar{u} + d\bar{d} - 2s\bar{s}|/\sqrt{6}$, and $|\phi_0\rangle = |u\bar{u} + d\bar{d} + s\bar{s}|/\sqrt{3}$. To leading order in isospin violation, we have

$$|\pi^0\rangle = |\phi_0\rangle + \varepsilon (\cos \theta |\phi_0\rangle - \sin \theta |\phi_8\rangle) + \varepsilon' (\sin \theta |\phi_0\rangle + \cos \theta |\phi_8\rangle)$$

where $|\eta\rangle = \cos \theta |\phi_8\rangle - \sin \theta |\phi_0\rangle + O(\varepsilon)$, and $|\eta'\rangle = \sin \theta |\phi_8\rangle + \cos \theta |\phi_0\rangle + O(\varepsilon')$. Expanding QCD to leading order in $1/N_c$ moments, and quark masses permits the construction of a low-energy, effective Lagrangian in which the pseudoscalar meson octet and singlet states

$$\hat{H}_{\text{eff}} |B^-\rangle = G_F \sqrt{2} V_{ub} V^*_td (if_\pi F_{B^-} |\phi_3\rangle (m^2_{\pi^-}) a_1 + if_\pi^{(u)} F_{B^-} (m^2_{\pi^0}) a_2) - V_{tb} V^*_td$$

$$\times (if_\pi F_{B^-} |\phi_3\rangle (m^2_{\pi^-}) (a_4 + a_{10}) + \frac{2m^2_{\pi^-}}{(m_u + m_d)(m_b - m_u)} (a_6 + a_8)) - if_\pi^{(u)} F_{B^-} (m^2_{\pi^0})$$

$$\times (a_4 + \frac{3}{2}(a_7 - a_9) - \frac{1}{2} a_{10} + \frac{m^2_{\pi^-}}{m_0 (m_b - m_d)(m_b - m_d)}).$$

The transition form factors are given by $F_{B^-}(q^2) = (m^2_{\pi^-} - m^2_{\pi^0}) F_{0}^{B \to \pi}(0)/(1 - q^2 / M_{0^+}^2)$, where we use $F_{0}^{B \to \pi}(0) = 0.33$ and $M_{0^+} = 5.73$ GeV as per Refs. [10,18]. Also $F_{B_{\phi_3}} = F_{B_{\phi_3}}/\sqrt{2}$, $F_{B_{\phi_0}} = F_{B_{\phi_0}}/\sqrt{6}$, and $F_{B_{\phi_0}} = F_{B_{\phi_3}}/\sqrt{3}$. In the presence of isospin violation, the $B^- \to \pi^- \phi_3$ amplitude is no longer purely $I = 2$. However, if $\pi^0 - \eta, \eta'$ mixing is neglected, $\bar{A}^{+0} + 2\bar{A}^{00} = \sqrt{2}\bar{A}^{-0}$, from Eq. [3], is still satisfied, as we ignore the small mass differences $m_{\pi^0} - m_{\phi_3}$ and $m_{B^-} - m_{B^0}$. Now with $\pi^0 - \eta, \eta'$ mixing,
\[ A^0 = \langle \pi^- \phi_3 | \mathcal{H}_{\text{eff}} | B^- \rangle + \varepsilon_8 \langle \pi^- \phi_8 | \mathcal{H}_{\text{eff}} | B^- \rangle + \varepsilon_0 \langle \pi^- \phi_0 | \mathcal{H}_{\text{eff}} | B^- \rangle \]  
\[ \overline{A}^{00} = \langle \phi_3 \phi_3 | \mathcal{H}_{\text{eff}} | B^0 \rangle + 2 \varepsilon_8 \langle \phi_3 \phi_8 | \mathcal{H}_{\text{eff}} | B^0 \rangle + 2 \varepsilon_0 \langle \phi_3 \phi_0 | \mathcal{H}_{\text{eff}} | B^0 \rangle , \]  
(8a)  
(8b)

where \( \varepsilon_8 \equiv \varepsilon \cos \theta + \varepsilon' \sin \theta \), \( \varepsilon_0 \equiv \varepsilon' \cos \theta - \varepsilon \sin \theta \), and further details appear in Ref. [13].

The \( B \to \pi \pi \) amplitudes now satisfy

\[ \overline{A}^{++} + 2 \overline{A}^{00} - \sqrt{2} \overline{A}^{-0} = 4 \varepsilon_8 \langle \phi_3 \phi_8 | \mathcal{H}_{\text{eff}} | B^0 \rangle + 4 \varepsilon_0 \langle \phi_3 \phi_0 | \mathcal{H}_{\text{eff}} | B^0 \rangle \]  
\[ - \sqrt{2} \varepsilon_8 \langle \pi^- \phi_8 | \mathcal{H}_{\text{eff}} | B^- \rangle - \sqrt{2} \varepsilon_0 \langle \pi^- \phi_0 | \mathcal{H}_{\text{eff}} | B^- \rangle , \]  
(9)

and thus the previous triangle relation becomes a quadrilateral. Numerical results in the factorization approximation for the reduced amplitudes \( A_R \) and \( \overline{A}_R \), where \( \overline{A}_R^{00} \equiv 2 \overline{A}_R^{00} / (G_F / \sqrt{2}) i V_{ub} V_{ud}^* \), \( \overline{A}_R^{++} \equiv \overline{A}_R^{++} / (G_F / \sqrt{2}) i V_{ub} V_{ud}^* \), and \( \overline{A}_R^{-0} \equiv \sqrt{2} A^{-0} / (G_F / \sqrt{2}) i V_{ub} V_{ud}^* \), with \( N_c = 2, 3, \infty \) and \( k^2/m_b^2 = 0.3, 0.5 \) are shown in Fig. [4].

Here the parameter \( N_c \) defines different hadronic models; \( N_c = 2, 3 \) bound the value favored from fits to measured branching ratios [12]. Following Ref. [4], the determination of \( \text{Im} r_{\pi^+ \pi^-} \) yields \( \sin 2\alpha \), modulo discrete ambiguities in \( z \) and \( \pi \) as in Eq. [4].

However, \( \sin 2\alpha \) can be determined uniquely through a comparison with \( \sin 2\alpha \) from \( \text{Im} r_{\pi^0 \pi^0} \), as only one pair of the \( \sin 2\alpha \) extracted from \( \text{Im} r_{\pi^+ \pi^-} \) and \( \text{Im} r_{\pi^0 \pi^0} \) likely match. As \( |A_2|/|A_2| \neq 1 \) in the presence of isospin violation, we have retained this explicit factor in the last equality of Eq. [4] in order to extract \( \sin 2\alpha \) as accurately as possible.

The values of \( \sin 2\alpha \) extracted from the amplitudes in the factorization approximation with \( N_c \) and \( k^2/m_b^2 = 0.5 \) are shown in Table [4] for a variety of input values of \( \sin 2\alpha \) — the results for \( k^2/m_b^2 = 0.3 \) are similar and have been omitted. In the presence of \( \pi^0 - \eta, \eta' \) mixing, the \( A_R^{++}, A_R^{-0}, \) and \( A_R^{00} \) amplitudes obey a quadrilateral relation as per Eq. [2], so that the amplitudes of interest need no longer form triangles. Consequently, the values of \( \sin 2\alpha \) extracted from \( \text{Im} r_{\pi^+ \pi^-} \) and \( \text{Im} r_{\pi^0 \pi^0} \) can not only differ markedly from the value of \( \sin 2\alpha \) input but also need not match. The incurred error in \( \sin 2\alpha \) increases as the value to be extracted decreases; the structure of Eq. [4] suggests this, for as \( \sin 2\alpha \) decreases the quantity \( \text{Im}((1 - \pi)/(1 - z)) \) becomes more important to determining the extracted value.

It is useful to constrain the impact of the various isospin-violating effects. The presence of \( \Delta I = 3/2 \) penguin contributions, be they from \( m_u \neq m_d \) or electroweak effects, shift the extracted value of \( \sin 2\alpha \) from its input value, yet the “matching” of the \( \sin 2\alpha \) values in \( \text{Im} r_{\pi^+ \pi^-} \) and \( \text{Im} r_{\pi^0 \pi^0} \) is unaffected. The mismatch troubles seen in Table [4] are driven by \( \pi^0 - \eta, \eta' \) mixing, though the latter shifts the values of \( \sin 2\alpha \) in \( \text{Im} r_{\pi^+ \pi^-} \) as well. Picking the closest matching values of \( \sin 2\alpha \) in the two final states also picks the solutions closest to the input value; the exceptions are noted in Table [4]. The matching procedure can also yield the wrong strong phase; in case b) of Table [4] with \( N_c = 3, \infty \), the triangles of the chosen solutions “point” in the same direction, whereas they actually point oppositely.

If \( |A_{00}| \) and \( |\overline{A}_{00}| \) are small [4] the complete isospin analysis may not be possible, so that we examine the utility of the bounds proposed in Ref. [20] on the strong phase \( 2\delta_{\text{true}} \equiv \)
\[ \arg((1 - z)/(1 - z)) \text{ in Eq. } [\text{I}]. \] The bounds \(2\delta_{GQ1}\) and \(2\delta_{GQII}\) given by Eqs. 2.12 and 2.15, respectively, in Ref. [20] follow from Eq. [3], and thus can be broken in the presence of isospin violation. As shown in Table [I], the bounds typically are broken, and their efficacy does not improve as the value of \(\sin 2\alpha\) to be reconstructed grows large.

To conclude, we have considered the role of isospin violation in \(B \to \pi\pi\) decays and have found the effects to be significant. Most particularly, the utility of the isospin analysis in determining \(\sin 2\alpha\) strongly depends on the value to be reconstructed. The error in \(\sin 2\alpha\) from a \(\text{Im} \pi^+\pi^-\) measurement can be 50\% or more for the small values of \(\sin 2\alpha\) currently favored by phenomenology [10,15,21]; however, if \(\sin 2\alpha\) were near unity, the error would decrease to less than 10\%. The effects found arise in part because the penguin contribution in \(B^0 \to \pi^+\pi^-\), e.g., is itself small; we estimate \(|P|/|T| < 9\%|V_{tb}V_{td}^*|/|V_{ub}V_{ud}^*|\). Relative to this scale, the impact of \(\pi^0\)-\(\eta, \eta'\) mixing is significant. Yet, were the penguin contributions in \(B \to \pi\pi\) larger, the isospin-violating effects considered would still be germane, for not only would the \(\Delta I = 3/2\) penguin contributions likely be larger but the \(B \to \pi\eta\) and \(B \to \pi\eta'\) contributions could also be larger as well [22]. To conclude, we have shown that the presence of \(\pi^0\)-\(\eta, \eta'\) mixing breaks the triangle relationship, Eq. [3] usually assumed [1] and can mask the true value of \(\sin 2\alpha\).

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TABLE I. Strong phases and inferred values of $\sin 2\alpha$ from amplitudes in the factorization approximation with $N_c$ and $k^2/m_b^2 = 0.5$. The strong phase $2\delta_{\text{true}}$ is the opening angle between the $\overline{A}_R^{+_-}$ and $A_R^{+_-}$ amplitudes in Fig. 1, whereas $2\delta_{\text{GL}}$ is the strong phase associated with the closest matching $\sin 2\alpha$ values, denoted $(\sin 2\alpha)_{\text{GL}}$, from $\text{Im}\frac{\pi^+}{\pi^-}/\text{Im}\frac{\pi^0}{\pi^0}$, respectively. The bounds $|2\delta_{\text{GQI}}|$ and $|2\delta_{\text{GQII}}|$ on $2\delta_{\text{true}}$ from Eqs. 2.12 and 2.15 of Ref. [20] are also shown. All angles are in degrees. We input a) $\sin 2\alpha = 0.0432$ [10, 13], b) $\sin 2\alpha = -0.233$ ($\rho = 0.2, \eta = 0.35$) [21], and c) $\sin 2\alpha = 0.959$ ($\rho = -0.12$). * The matching procedure fails to choose a $\sin 2\alpha$ which is as close to the input value as possible. † The discrete ambiguity in the strong phase is resolved wrongly.

| case | $N_c$ | $2\delta_{\text{true}}$ | $|2\delta_{\text{GQI}}|$ | $|2\delta_{\text{GQII}}|$ | $|2\delta_{\text{GL}}|$ | $(\sin 2\alpha)_{\text{GL}}$ |
|------|------|------------------|------------------|------------------|------------------|------------------|
| a    | 2    | 24.4             | 26.1             | 15.8             | 16.6             | -0.0900/-0.0221  |
| a    | 3    | 24.2             | 16.9             | 16.1             | 16.2             | -0.0926/0.107    |
| a    | $\infty$ | 23.8           | 59.4             | 25.1             | 23.6             | 0.0451/0.394     |
| b    | 2    | 19.6             | 23.4             | 12.1             | 12.9             | -0.343/-0.251    |
| b    | 3    | 19.4             | 13.5             | 12.9             | 13.0             | -0.719/-0.855(*) |
| b    | $\infty$ | 19.2           | 59.9             | 23.6             | 0.76             | -0.550/-0.814(*, †) |
| c    | 2    | 28.3             | 36.5             | 20.4             | 21.0             | 0.917/0.915      |
| c    | 3    | 28.0             | 24.0             | 19.1             | 19.0             | 0.905/0.952      |
| c    | $\infty$ | 28.3           | 36.5             | 20.4             | 21.0             | 0.917/0.915      |
FIG. 1. Reduced amplitudes in $B \to \pi\pi$ in the factorization approximation with $[N_c, k^2/m_b^2]$ for a) $[2,0.5]$, b) $[3, 0.5]$ (solid line) and $[3, 0.3]$ (dashed line), and c) $[\infty,0.5]$.