CP violating phase sum rule $\delta_q + \delta_l = 0$ for CKM and PMNS matrices

Junxing Pan$^{1,∗}$, Jin Sun$^{2,†}$, Xiao-Dong Ma$^{3,‡}$, and Xiao-Gang He$^{3,4,§}$

$^1$School of Physics and Information Engineering, Shanxi Normal University, Linfen 041004, China
$^2$Tsung-Dao Lee Institute, and School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China
$^3$Department of Physics, National Taiwan University, Taipei 10617, Taiwan and
$^4$Physics Division, National Center for Theoretical Sciences, Hsinchu 30019, Taiwan

The non-zero Dirac phases $\delta_q$ and $\delta_l$ in the CKM and PMNS mixing matrices signify CP violation. In general they are independent. Experimental data show, however, that in the original KM parametrization for the mixing matrix, the sum $\delta_q + \delta_l$ is close to zero with $\delta_q$ to be approximately $\pi/2$. The KM parametrization may have provided some hints that these phases are actually related and CP is maximally violated. We show that this sum rule can be accommodated in models with spontaneous CP violation where both phases originate from a non-trivial common spontaneous CP violating maximized phase in the Higgs potential. We find some interesting phenomenological consequences for flavor changing neutral current and CP violation for such a model. In particular, data from $B_s - \bar{B}_s$ mixing provide very strong constraints on the mass scale for the new neutral scalars in the model, yet the model still allows the electric dipole moments of electron and neutron to reach to their current upper bounds. The model can be tested by near future experiments.

Introduction

There are mixings for quarks and leptons. These mixings are described by the Cabbibo-Kobayashi-Maskawa (CKM) matrix $V_{\text{CKM}}$ and Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix $V_{\text{PMNS}}$ in the following interaction Lagrangian

$$L = -\frac{g}{\sqrt{2}} \bar{U}_L V_{\text{CKM}} \gamma^\mu D_{L} W_{\mu}^+ - \frac{g}{\sqrt{2}} \bar{E}_{L} V_{\text{PMNS}} \gamma^\mu \nu_L W_{\mu}^+ + \text{H.C.} \ . \quad (1)$$

For three generations, $V_{\text{CKM}}$ and $V_{\text{PMNS}}$ are $3 \times 3$ unitary matrices and each can be parameterized by 3 rotation angles, $\theta_{12}, \theta_{23}$ and $\theta_{13}$ in the convention used by the Particle Data Group [6, 7], and a CP violating phase $\delta$, referred to as a Dirac phase. We will use a superscript $q$ and $l$ to indicate the angles and phases for quark and lepton mixings.

If neutrinos are Dirac particles, $V_{\text{PMNS}}$ matrix is similar to $V_{\text{CKM}}$ in form. If neutrinos are Majorana particles, $V_{\text{PMNS}}$ is, in general, modified by multiplying a diagonal matrix $P = \text{diag}(1, e^{i\alpha_1/2}, e^{i\alpha_2/2})$ with two additional CP Majorana phases $\alpha_{1,2}$ from right to the pure Dirac neutrino case. The values of rotation angles and the phases in the quark and lepton sectors are parametrization convention dependent.

The mixings in the quark and lepton sectors may or may not be related. In the literature, some attempts have been made to link them together such as complementarity of the mixing angles studied in [8]. Here we would like to suggest that the CP violating phases of these two sectors are related and the CP violating Dirac phases reach their maximal up to a sign, that is $\delta^{q,l} = \pm \pi/2$.

There are a lot of information about quark and lepton mixing parameters. The values for the rotation angles and phases are usually given in the Particle Data Group (PDG) parameterization, for example quark and lepton mixing from the recent UTfit and NuFit Collaborations [9, 10], respectively. Concerning CP violating phases $\delta_{\text{PDG}}^q$ and $\delta_{\text{PDG}}^l$, the best (3$\sigma$ ranges) are given by $\delta_{\text{PDG}}^q / \pi = 0.3717$ ($0.3606 \sim 0.3828$) for quark mixing, and $\delta_{\text{PDG}}^l / \pi = -0.772$ ($-1.200 \sim -0.017$) for lepton mixing with normal hierarchy (NH) ( and $\delta_{\text{PDG}}^l / \pi = -0.433$ ($-0.861 \sim -0.067$) for inverted hierarchy (IH)). The CP violating phase in the quark sector is away from $\pi/2$. In the lepton sector, the
CP violating phase is consistent with $-\pi/2$. The rotation angles and phases in the two sectors do not seem to show correlations. Note that the current data allow the intriguing possibility that, for lepton mixing to have $\theta_{23}^e$ and $\delta_{\text{PDG}}^e$ to be $\pi/4$ and $-\pi/2$ (or $3\pi/2$), respectively.

The specific values of the rotation angles and phases are parametrization convention dependent. Let us translate the values of rotation angles and CP violating phases into the original KM parameterization for quark mixing, given by \[ \theta_{\text{KM}} = \left( \begin{array}{ccc} c_1^2 & -s_1^2 e^{i\delta_1} & -s_1^2 s_3 e^{i\delta_3} \\ s_1^2 c_2 & c_1 c_2 c_3 - s_2 s_4 e^{i\delta_4} & c_1 c_2 s_3 + s_2 s_4 e^{i\delta_4} \\ s_1^2 s_2 & c_1 s_2 c_3 - s_2 s_4 e^{i\delta_4} & c_1 s_2 s_3 - s_2 s_4 e^{i\delta_4} \end{array} \right), \]

where $s_j = \sin \theta_j$ and $c_j = \cos \theta_j$.

Using the values obtained by UTfit and NuFit collaborations [9,11], we have for quark mixing parameters given by

\[ \text{KM:} \quad s_1^q = 0.2520, \quad (3\sigma : 0.2240, 0.2260), \quad s_2^q = 0.03863, \quad (3\sigma : 0.03751, 0.03974), \]
\[ s_3^q = 0.01633, \quad (3\sigma : 0.01584, 0.01683), \quad \delta_{\text{KM}}^q/\pi = 0.4950, \quad (3\sigma : 0.4780, 0.5120), \]

and for lepton mixing parameters given by

\[ \text{KM – NH:} \quad s_1^l = 0.5705, \quad (3\sigma : 0.5383, 0.6048), \quad s_2^l = 0.8463, \quad (3\sigma : 0.4533, 0.9101), \]
\[ s_3^l = 0.2622, \quad (3\sigma : 0.2372, 0.2885), \quad \delta_{\text{KM}}^l/\pi = -0.7433, \quad (3\sigma : -1, -0.2546), \]
\[ \text{KM – IH:} \quad s_1^l = 0.5706, \quad (3\sigma : 0.5385, 0.6050), \quad s_2^l = 0.7175, \quad (3\sigma : 0.4603, 0.8989), \]
\[ s_3^l = 0.2634, \quad (3\sigma : 0.2383, 0.2897), \quad \delta_{\text{KM}}^l/\pi = -0.4222, \quad (3\sigma : -0.8586, -0.0658). \]

We see that in the KM parameterization, the phases are closer in size compared with those in the PDG parameterization and different in sign and $\delta_{\text{KM}}^q$ is very close to $\pi/2$, particularly for IH case. As mentioned before that the current data allow the intriguing possibility that, in the neutrino mixing, $\theta_{23}$ and $\delta_{\text{PDG}}$ to be $\pi/4$ and $-\pi/2$ (or $3\pi/2$). This has generated extensive efforts to realize such special scenarios which give some guidance to model buildings [12]. It has been pointed out that, in fact parameterization with a rotation angle to be $\pi/4$ and the CP violating phase to be $-\pi/2$ is not unique to PDG parameterization. The KM parameterization with $\theta_{23}$ and $\delta_{\text{PDG}}$ to be $\pi/4$ and $-\pi/2$ is actually equivalent to that in the PDG parameterization with $\theta_{23}$ and $\delta_{\text{PDG}}$ to be $\pi/4$ and $-\pi/2$ (or $3\pi/2$) [13].

It is interesting to note that the CP violating phases in the KM parameterization satisfy $\delta_{\text{KM}}^q + \delta_{\text{KM}}^l = 0$ within error bars and the central value of $\delta_{\text{KM}}^l$ is $\pi/2$. This might be a hint as a possible relation between CP violating phases in quark and lepton mixing matrices and CP is violated maximally in both quark and lepton sectors.

**Model realization of $\delta_{\text{q}}^l + \delta_{\text{l}}^q = 0$ sum rule**

We now show that the sum rule of $\delta_{\text{q}}^l + \delta_{\text{l}}^q = 0$ can be realized in a multi-Higgs model which can solve the strong CP problem by Peccei-Quinn (PQ) symmetry with spontaneous CP violation. In addition, we can also relate the invisible axion PQ symmetry scale to the see-saw scale for small neutrino mass. In this model, beside the usual SM 3 generations of fermions $Q_L : (3, 2, 1/6), U_R : (3, 1, 2/3), D_R : (3, 1, -1/3), L_L : (1, 2, -1/2)$ and $E_R : (1, 1, -1)$, we also introduce 3 right handed neutrinos $\nu_R : (1, 1, 0)$ to facilitate seesaw mechanism for neutrino masses. Here the numbers in the brackets indicate the SM gauge group $SU(3)_C \times SU(2)_L \times U(1)_Y$ quantum numbers. It has been shown that in order to have spontaneous CP violation with PQ symmetry at least three Higgs doublets transforming as $(1,2,-1/2)$: $\phi_i = e^{i\theta_i} H_i = e^{i\theta_i} ((v_i + R_i + i A_i)/\sqrt{2}, h_i^-)^T$ with $i = 1, 2, 3$ and one complex Higgs singlet $L_L : (1, 1, 0): \tilde{S} = e^{i\theta_s} S = e^{i\theta_s} (v_s + R_s + i A_s)/\sqrt{2}$ are needed [14,15]. We will assume that $v_s \gg v_{1,2,3}$ so that the axion is invisible and also the seesaw mechanism is in effective. With the Higgs multiplets given, it has been shown that it is possible to have spontaneous CP violation with only one independent phase $\delta_{\text{sp}} = \theta_1 - \theta_2$ in the Higgs potential. We will not go into details here for the Higgs potential analysis.
For our purpose, we assign the following PQ charges to the Higgs fields and the fermion fields, $Q_L : 0$, $U_R : +1$, $D_R : +1$, $L_L : 0$, $\nu_R : +1$, $E_R : +1$, $\phi_{1,2} : +1$, $\phi_u = \phi_3 : -1$, $\bar{S} : +2$. With the above PQ charges for the particles, the Yukawa couplings are given by

$$L_Y = -\bar{Q}_L Y_u \phi_3 U_R - \bar{Q}_L (Y_{d1} \tilde{\phi}_1 + Y_{d2} \tilde{\phi}_2) D_R - \bar{L}_L Y_e \phi_3 \nu_R - \bar{L}_L (Y_{e1} \tilde{\phi}_1 + Y_{e2} \tilde{\phi}_2) E_R - \frac{1}{2} \nu_R^c \tilde{S} \nu_R + H.C., \quad (5)$$

where $\tilde{\phi}_i = -i \sigma_2 \phi_i^*$.

Absorbing the phases $\theta_3$, $-\theta_s/2$, $-(\theta_3 + \theta_s/2)$, $-\theta_1$ and $-(\theta_1 + \theta_3 + \theta_s/2)$ into redefinitions of $U_R$, $\nu_R$, $L_L$, $D_R$ and $E_R$, respectively, and writing the fermion mass terms in the form: $L_m = -\overline{D}_L M_d D_R - \overline{U}_L M_u U_R - \overline{E}_L M_e E_R - \overline{T}_L M_D \nu_R - \frac{1}{2} \overline{\nu_R} M_R \nu_R$, we have

$$M_d = M_{d1} + M_{d2} e^{i \delta_{sp}}$, $M_e = M_{e1} + M_{e2} e^{i \delta_{sp}}$, $M_{ai} = Y_{ai} \frac{v_i}{\sqrt{2}}$, $M_u = Y_u \frac{v_3}{\sqrt{2}}$, $M_D = Y'_u \frac{v_3}{\sqrt{2}}$, $M_R = Y'_s \frac{v_s}{\sqrt{2}}$, $\quad (6)$$

The light seesaw neutrino mass matrix is given by $M_{\nu} = -M_D M_R^{-1} M_D^T$.

Working in the basis where $M_u$ and $M_D$ are already diagonalized, the mass matrices for the down quark and charged lepton can be written as

$$M_d = V_{dL} \hat{M}_d V_{dR}^T, \quad M_e = V_{eL}^\dagger \hat{M}_e V_{eR}^T, \quad (7)$$

where $\hat{M}_i$ are diagonal matrices whose entries are the eigen-masses. Comparing with eq. (1), we obtain

$$V_q = V_{dL}^\dagger, \quad V_l = V_{eL}^\dagger. \quad (8)$$

We now discuss how to link the Dirac phases in the CKM and PMNS matrices with the spontaneous CP violating phase $\delta_{sp}$. To achieve this, an additional assumption that $V_{\nu}^{d,e,c}$ to be unit matrices is needed. With this assumption, we have

$$V_q \hat{M}_d = (\text{Re} V_q + i \text{Im} V_q) \hat{M}_d = (M_{d1} + M_{d2} e^{i \delta_{sp}}), \quad V_{lL}^\dagger \hat{M}_e = (\text{Re} V_{lL}^\dagger + i \text{Im} V_{lL}^\dagger) \hat{M}_e = (M_{e1} + M_{e2} e^{i \delta_{sp}}). \quad (9)$$

The above allows us to identify: $\delta_q = \delta_{sp}$, $\delta_l = -\delta_{sp}$. With the help of this assumption, we therefore have obtained the desired sum rule: $\delta_q + \delta_l = 0$. One may argue that CP is maximally violated in the Higgs potential so that $\delta_{sp}$ is $\pi/2$.

We should comment that although to obtain the desired solutions for the CP violating phases additional assumptions have to be made, the fact that there are solutions which can accommodate experimental data shown in the KM parameterization linking the phases in quark and lepton sectors makes it interesting to study related phenomenological consequences further.

**New Higgs mediated interactions**

There are additional Higgs bosons in the model which bring in new interactions. To obtain new Higgs interactions, it is convenient to work in the basis where un-physical Higgs fields have been removed and the axion $a$ identified. The un-physical Higgs bosons are the Goldstone fields $h_w$ and $h_z$ “eaten” by $W$ and $Z$ bosons. The physical fields, $a_{1,2}$, $a$ and $H_1^0$ related to the original fields are given by [16]

$$
\begin{pmatrix}
A_1 \\
A_2 \\
A_3 \\
A_4 \\
h_1^- \\
h_2^- \\
h_3^-
\end{pmatrix}
= \begin{pmatrix}
v_2/v_1 & -v_1 v_3 / v_1 N_a & v_1 / v & v_1 v_3^2 / v N_a \\
-1 & -v_1 v_3 / v_1 N_a & v_2 / v & v_2 v_3^2 / v N_a \\
0 & v_1 v_3 / v_1 N_a & v_3 / v & -v_3^2 v_3 / v N_a \\
0 & v_1 v_3 / v_1 N_a & v_3 / v & v_3^2 v_3 / v N_a \\
v_2 / v_1 & v_1 v_3 / v_1 N_a & v_1 / v & v_2 / v \\
-1 & -v_1 v_3 / v_1 N_a & v_2 / v & v_2 v_3^2 / v N_a \\
0 & v_1 v_3 / v_1 N_a & v_3 / v & -v_3^2 v_3 / v N_a \\
0 & v_1 v_3 / v_1 N_a & v_3 / v & v_3^2 v_3 / v N_a \\
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
a \\
h_z \\
h_1^- \\
h_2^- \\
h_3^-
\end{pmatrix}.
$$

$$
\begin{pmatrix}
h_1^- \\
h_2^- \\
h_3^-
\end{pmatrix}
= \begin{pmatrix}
v_2 / v_1 & v_1 v_3 / v_1 N_a & v_1 / v \\
-1 & -v_1 v_3 / v_1 N_a & v_2 / v \\
0 & v_1 v_3 / v_1 N_a & v_3 / v \\
\end{pmatrix}
\begin{pmatrix}
H_1^- \\
H_2^- \\
h_w
\end{pmatrix}, \quad (10)$$
where \( v^2 = v_1^2 + v_2^2 + v_3^2 \), \( v_{12}^2 = v_1^2 + v_2^2 \), and \( N_a^2 = (v_2^2 v_3^2 + v_1^2 v_2^2) \). \( a_{1,2} \) and \( H_{1,2}^- \) are the physical degrees of freedom for the Higgs fields. With the same rotation as that for the neutral pseudoscalars, the neutral scalar Higgs fields \( (R_1, R_2, R_3)^T \) become \( (H_1^0, H_2^0, H_3^0, H_4^0)^T \). Since the invisible axion scale \( v_a \) is much larger than the electroweak scale, to a very good approximation, \( N_a \approx v v_a \).

Note that \( H_0^0, a_1 \) and \( H_1^- \) are not yet the mass eigenstates. To find the mass eigenstates, one needs to further analyze the Higgs potential. They are approximately mass eigenstates if the mixings are small. In this limit, \( H_3^0 \) is the SM-like Higgs boson. The interacting terms of neutral Higgs boson with fermions are

\[
L_N = -\bar{U}_L M_u U_R \left[ \frac{\nu_2 v_1 v_3}{v_3 N_a} (H_2^0 + i a_2) + H_3^0 - \frac{v_2^2}{N_a} (H_4^0 + i a) \right] \\
- \left( \bar{D}_L M_d D_R + \bar{E}_L M_e E_R \right) \left[ \frac{v_2 v_1 (H_1^0 - i a_1)}{v_1 v_{12}} - \frac{v_3 v_1 v_2}{v_{12} N_a} (H_2^0 - i a_2) + H_3^0 + \frac{v_2^2}{N_a} (H_4^0 - i a) \right] \\
+ \left( \bar{D}_LV_L^\dagger q_1 M_d D_R + \bar{E}_LV_L^\dagger q_2 M_e E_R \right) \left[ \frac{v_2 v_{12}}{v_1 v_{12}} (H_1^0 - i a_1) + H.C. \right].
\]

(11)

where we have decomposed \( V_i = V_{i1} + V_{i2} e^{i \delta_i} \). The values of \( V_{11} \) and \( V_{12} \) can be read off from eq. (2).

In the above, we have not displayed the Yukawa couplings involving \( v_R \) which has some components of light neutrinos, but the couplings are small. Furthermore, in the large \( v_a \) limit, the axion is invisible and also the seesaw mechanism works. The couplings of \( a_1 \) and \( H_3^0 \) to SM fermions are also small. Note that \( H_1^0 \) and \( a_1 \) can mediate flavor changing neutral current (FCNC) at tree level \[16\] \[17\]. We will use data to constrain the model parameters from FCNC interactions due to exchange of \( H_1^0 \) and \( a_1 \). Due to spontaneous CP violation, the Higgs potential will mix \( H_i^0 \) with \( a_i \) which also has important implications for CP violation and will be studied.

For definitiveness of numerical analysis, considering \( v_3 \) gives mass to top quark, \( v_{1,2} \) are related to down-type quark masses with the bottom quark having the mass compatible with the larger one, to make Yukawa couplings to be large but not to upset perturbative calculations, we assume that the largest Yukawa couplings are around 1. It is then natural to have \( v_2 \sim v, v_{12}/v_3 \sim m_b/m_t \). We also assume \( v_2 \sim v_1 \), which implies \( v_2/(v_1 v_{12}) \sim (1/v)(m_t/m_b) \) and \( v_{12}/(v_1 v_2) \sim (2/v)(m_t/m_b) \). If \( v_1 \neq v_2 \), the constraints obtained will be different. We will comment on this situation at the end of the numerical analysis.

**FCNC constraints**

The \( V_{q2,i} \) obtained from eq. (2) lead to FCNC only between the second and third generations which can cause \( B_s - \bar{B}_s \) mixing and \( \tau \rightarrow \mu \mu \bar{\nu} \). The FCNC interactions can lead to enhanced \( \tau \rightarrow \mu \gamma \) at loop level which gives the most stringent constraint on the scalar scale using data from lepton sector.

The one loop diagram generating \( \tau \rightarrow \mu \gamma \) is shown in Fig. 1(a). We find that the dominant contribution is from \( \tau \) propagator due to the enhanced Yukawa couplings. Neglecting small corrections of order \( O(m_\mu^2/m_\tau^2) \), we have

\[
\Gamma(\tau \rightarrow \mu \gamma) = \frac{\alpha_{em} m_\tau (s_2 s_3)^2}{64 \pi^4} \frac{m_1^2}{v_1^4} \left( 1 - \left( \frac{v_2}{v_1} \right) \right)^2 \left[ \frac{m_\tau^2}{m_{a_1}^2} \left( \frac{m_\tau^2}{m_{a_1}^2} + \frac{5}{3} \right) \right] - \frac{m_\tau^2}{m_{H_1}^2} \left[ \left( \frac{m_\tau^2}{m_{H_1}^2} + \frac{4}{3} \right) \right]^2.
\]

(12)

where \( \alpha_{em} \) is the fine structure constant.

Using the upper bound \( Br(\tau \rightarrow \mu \gamma)^{\text{exp}} < 4.4 \times 10^{-8} \) at 90% confidence level (CL) \[11\] with the central value of \( s_2^2 = 0.8463 \) for the NH case, we obtain the excluded parameter space in the \( m_{a_1} - m_{H_1} \) plane shown in the left panel of Fig. 3 in purple.

For the \( \tau \rightarrow \mu \mu \bar{\nu} \), it can take place at tree level as shown in Fig. 1 (b) via the exchange of \( H_1^0 \) and \( a_1 \). This process also receives comparable contributions from diagrams attaching the photon line in Fig. 1(a) to a muon pair. Currently the experimental upper bound for the branching ratio is \( Br(\tau \rightarrow \mu \mu \bar{\nu})^{\text{exp}} < 2.1 \times 10^{-8} \) at 90% CL \[11\]. Using this bound we have evaluated possible constraints on the masses of \( a_1 \) and \( H_1^0 \) shown in Fig. 3 in red color.
The enhanced coupling of $H_0^1$ and $a_1$ to leptons may also have impact on the anomalous magnetic dipole moment of muon $g - 2$. We have the one and two loop contributions from Fig. 1 (a) with the initial tauon replaced by the muon and Fig. 2 (a) with the identification that $\psi = \mu$, respectively. We find the 1-loop contribution with an intermediate $\tau$ is dominant over the 2-loop contributions by a factor of $O(10^3)$. As can be seen from Fig. 2 with low mass of order 180 GeV, it is possible to produce correction $\Delta a_\mu \sim (28.02 \pm 7.37) \times 10^{-10}$ to solve the muon $g-2$ anomaly problem. But this has been ruled out by other constraints.

We find the mass difference $\Delta M_{B_s}$ of the $B_s - \bar{B_s}$ system provides the most stringent constraint. The SM has a well predicted value for $\Delta M_{B_s}$ with $\Delta M_{B_s}^{SM} = (17.25 \pm 0.85) \, \text{ps}^{-1}$ which agrees with experimental data $\Delta M_{B_s}^{exp} = (17.757 \pm 0.021) \, \text{ps}^{-1}$ well. This means that any new physics contributions are constrained. We will allow the new physics contribution $\Delta M_{B_s}^{NP}$ and the SM prediction $\Delta M_{B_s}^{SM}$ in the $3\sigma$ allowed ranges. Exchanges of $H_0^1$ and $a_1$ can contribute to $\Delta M_{B_s}^{NP}$ at the tree level as shown in Fig. 1 (c). In the vacuum saturation approximation (VSA), we obtain $H_0^1$ and $a_1$ contributions to the mass splitting $\Delta M_{B_s}$ for $B_s - \bar{B_s}$ mixing as the following

$$
\Delta M_{B_s}^{NP} = \frac{1}{2} S_{3\r}^2 \left( \begin{array}{cc}
\frac{v}{v_1 v_2} & 0 \\
0 & \frac{v}{v_1 v_2}
\end{array} \right) \left\{ \frac{5}{12} \left( \frac{1}{m_{H_0^1}} - \frac{1}{m_{a_1}} \right) \frac{m_s^2 + m_b^2}{v^2} \frac{m_{B_s}^2}{(m_s + m_b)^2} B_S \\
- \left( \frac{1}{m_{H_0^1}} + \frac{1}{m_{a_1}} \right) \frac{m_s m_b}{v^2} \left[ \frac{m_{B_s}^2}{(m_s + m_b)^2} B_S + \frac{1}{6} B_V \right] \right\} f_{B_s}^2 m_{B_s},
$$

(13)

where $B_V$ and $B_S$ are the bag correction factors defined as via $19$: $\langle B_s | (\bar{b}_R \gamma_\mu P_L s)(\bar{b}_R \gamma_\mu P_L s) | B_s \rangle = (2/3) f_{B_s}^2 m_{B_s}^2 B_V$ and $\langle B_s | (\bar{b}_R \gamma_\mu P_L s)(\bar{b}_R \gamma_\mu P_L s) | B_s \rangle = -(5/12) f_{B_s}^2 m_{B_s}^2 B_S$. For numerical analysis, we take $B_V = 0.849$ and $B_S = 0.835$ with $f_{B_s} = 230$ MeV for the $B_s$ decay constant, and $m_b = 4.18$ GeV and $m_s = 93$ MeV for $b$ and $s$ quark masses.

In the orange region of Fig. 2 we display constraints from the above considerations. We find that the $B_s - \bar{B_s}$ mixing gives the most stringent constraint. The $H_0^1$ and $a_1$ masses are constrained to be larger than $O(1 \, \text{TeV})$. This makes discovery of $H_0^1$ and $a_1$ at the LHC difficult. But some of the parameter space for the allowed masses for $H_0^1$ and $a_1$ may be probed by a 100 TeV collider.

If $v_1 \neq v_2$, the constraint will be even stronger. As $\Delta M_{B_s}^{NP}$ is proportional to $p = \frac{v v_{12}}{v_1 v_2}$, when $v_1$ becomes not equal to $v_2$ with a fixed $v_{12}$, the value $p$ will become larger and result in a stronger constraint on the masses for $H_0^1$ and $a_1$. Therefore the constraint provided above represents the most conservative one.
Electron and neutron EDM

Due to CP violation in the Higgs potential, $H_{1,2,3}^0$ and $a_{1,2}$ mixing will be generated at tree level through terms in the potential such as $(H_1^0 H_2^0) e^{-i2\delta_{rr}}$, $(H_1^0 H_1^0)(H_1^0 H_2^0) e^{-i\delta_{rr}}$, $(H_1^0 H_2^0)(H_1^0 H_2^0) e^{-i\delta_{rr}}$ and $(H_1^0 H_2^0)(H_1^0 H_3^0) e^{-i\delta_{rr}}$. We will parameterize the mixing approximately by $H_{1}^{0}\rightarrow H_{1}^{0}+\kappa_{ij}a_{j}$ and $a_{i}\rightarrow a_{i}\mp\kappa_{ij}H_{j}^{0}$.

The mixing parameters $\kappa_{ij}$ are free parameters which depend on the parameters in the potential. If the mixing is mainly due to $a_{i}$ and $H_{j}$ mass mixing term $m_{ij}^{2}$, $\kappa_{ij}$ is given approximately by $m_{ij}^{2}/(m_{a_{j}}^{2}-m_{H_{i}}^{2})$ which we assume to be much smaller than 1. An interesting effect of such a mixing is that a non-zero electric dipole model (EDM) $d_{f}$ of a fermion $f$ will be induced at loop levels.

For the electron EDM (eEDM), the 1-loop contribution is similar to Fig. 1 (a) with the external $\tau$ and $\mu$ being substituted by the electron. However, the dominant contribution is from the 2-loop Barr-Zee type diagram [21] shown in Fig. 3 (a) with the $b$-quark and $\tau$ lepton circulating in the loop, we have

$$d_{e}^{2L}=\frac{eG_{\text{em}}}{96\pi^{3}}m_{e}[G(m_{b},e)+3G(m_{\tau},e)]\,,$$

where

$$G(m_{e})=2\frac{\kappa v_{1}^{2}}{v_{1}^{2}}\left(1-c_{e}^{2}\frac{v_{1}^{2}}{v_{2}^{2}}\right)\left[f\left(m_{b}^{2}/m_{a_{j}}^{2}\right)+g\left(m_{\tau}^{2}/m_{a_{j}}^{2}\right)-f\left(m_{b}^{2}/m_{H_{i}}^{2}\right)-g\left(m_{\tau}^{2}/m_{H_{i}}^{2}\right)\right],$$

with $c_{e}=c_{e}(\frac{v_{1}}{v_{2}})$ for $m=m_{b}(m_{\tau})$. The loop function $f(z)$ and $g(z)$ can be found in [10].

For the neutron EDM (nEDM), there are several contributions such as those from (a) the EDM $-\frac{\bar{q}_{i}^{0}\rho_{i}^{0}\gamma_{5}q_{F}}{4\pi^{2}}$, (b) the color EDM (cEDM) $-\frac{1}{2}\bar{q}_{i}^{0}g_{a}q^{T}A_{a}\gamma_{5}q^{A_{a},\mu\nu}$, and (c) the Weinberg operator $\frac{1}{4}C_{W}f^{abc}G_{\mu\nu}^{a}\tilde{G}_{b,\nu}^{b,\mu}G_{\beta}^{c,\mu}$ [22].

The nEDM from the above effective interactions are estimated to be [16]

$$d_{n}\approx\eta_{d}\left(\frac{4}{3}d_{d}-\frac{1}{3}d_{u}\right)_{\Lambda}+\eta_{f}\left(\frac{4}{9}d_{d}+\frac{2}{9}d_{u}\right)_{\Lambda}+\xi C_{W},$$

where $f_{\pi}=95$ MeV is the pion decay constant. The QCD running factors from the electroweak to the hadronic scale $\Lambda\sim1$ GeV are approximately $\eta_{d}\approx0.166,\eta_{f}\approx0.0117$, and $\xi\approx1.2 \times 10^{-4}$, respectively.

In our model, the dominant contribution is from 2-loop diagrams shown in Fig. 3 which contribute the EDM in (a), the cEDM in (b), and the Weinberg operator in (c), respectively. The 2-loop contributions to EDM and cEDM of up quark from the mixing of $H_{1}^{0}$ and $a_{1}$ vanish, i.e., $d_{u} = f_{u} = 0$. Then we have the following compatible contributions

$$d_{e}^{2L}=\frac{eG_{\text{em}}}{288\pi^{3}}m_{d}[G(m_{b},d)+3G(m_{\tau},d)],$$

$$f_{d}^{2L}=-\frac{\alpha_{s}}{64\pi^{3}}m_{d}G(m_{b},d),$$

$$C_{W}^{2L}=-\frac{1}{4\pi^{2}}\frac{\kappa v_{1}^{2}}{v_{1}^{2}}\left(1-(e_{3}^{0})^{2}v_{1}^{2}/v_{2}^{2}\right)^{2}\left[h\left(m_{b}^{2}/m_{a_{j}}^{2}\right)-h\left(m_{\tau}^{2}/m_{H_{i}}^{2}\right)\right].$$

The loop function $h(z)$ can be also found in [16].

In the right panel of Fig. 2 we show the cEDM in purple and nEDM in orange as the function of the CP violating parameter $\kappa$. The solid lines represent the current experimental limits, in which $d_{e}^{\text{exp}}<1.1 \times 10^{-29}e\text{ cm}$ [23] and $d_{n}^{\text{exp}}<1.8 \times 10^{-26}e\text{ cm}$ [24] at 90% CL. The other different types of lines represent the different choices of $m_{a_{j}}$ and
allowed by the $B_s - \bar{B}_s$ mixing constraint. One can see, when $|\kappa|$ runs from $10^{-7}$ to $10^{-4}$, the eEDM and nEDM both get improved by several orders of magnitude relative to the SM predictions where $d_{e}^{\text{SM}} \leq O(10^{-38})$ e cm \[25\] and $d_{n}^{\text{SM}} \sim O(10^{-32})$ e cm \[26\], which could be reached by future EDM experiments to test such possibilities.

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