

Spontaneous CP violating phase as the CKM matrix phase

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Received: 17 August 2007 / Revised version: 8 October 2007 /

Published online: 8 January 2008 – © Springer-Verlag / Società Italiana di Fisica 2008

Abstract. We propose that the CP violating phase in the CKM mixing matrix is identical to the CP phases responsible for the spontaneous CP violation in the Higgs potential. A multi-Higgs model with Peccei–Quinn (PQ) symmetry is constructed to realize this idea. The CP violating phase does not vanish when all Higgs masses become large. In general, here are flavor changing neutral current (FCNC) interactions mediated by neutral Higgs bosons at the tree level. However, unlike general multi-Higgs models, the FCNC Yukawa couplings are fixed in terms of the quark masses and CKM mixing angles. Implications for meson–anti-meson mixing, including recent data on D – \bar{D} mixing, and the electric dipole moment (EDM) of the neutron are studied. We find that the neutral Higgs boson masses can be at the order of one hundred GeV. The neutron EDM can be close to the present experimental upper bound.

1 Introduction

The origin of CP violation is one of the outstanding problems of modern particle physics. There have been several experimental measurements of CP violation [1]. All of them are consistent with the Cabibbo–Kobayashi–Maskawa (CKM) model [2, 3], where the source of CP violation comes from the phase [3] δ_{KM} in the CKM mixing matrix for quarks. A successful model of CP violation at the leading order should have the successful features of the CKM model. It is important to understand the origin of CP violation. An interesting proposal due to Lee was that CP is spontaneously violated [4, 5]. The popular Weinberg model [6, 7] of spontaneous CP violation has problems [8–11] with the data and has been decisively ruled out by CP violating measurement in B decays [1]. Spontaneous CP violation in left–right models has also been ruled out for the same reason [12]. In this work we restore the idea that CP is broken spontaneously and the phase δ_{KM} is the same as the phase δ_{spon} that causes spontaneous CP violation in the Higgs potential. We construct some examples of such models that realize this idea. The main difference of our models lies in how the CP violating phase in the CKM matrix is identified [13, 14].

Let us start by describing how a connection between δ_{KM} and δ_{spon} can be made. It is well known that to have spontaneous CP violation, one needs two or more Higgs doublets ϕ_i . Consider the following Yukawa couplings with multi-Higgs doublets:

$$L_Y = \bar{Q}_L(\Gamma_{u1}\phi_1 + \Gamma_{u2}\phi_2)U_R + \bar{Q}_L\Gamma_d\tilde{\phi}_d D_R + \text{h.c.}, \quad (1)$$

where Q_L , U_R and D_R are the left-handed doublet, right-handed up and right-handed down quarks, respectively. Generation indices are suppressed. $\tilde{\phi}_d = -i\sigma_2\phi_d^*$ and ϕ_d may be one of the $\phi_{1,2}$ or another doublet Higgs field. The Yukawa couplings $\Gamma_{u1,u2,d}$ must be real if CP is only violated spontaneously.

The Higgs doublets when expressed in terms of the component fields and their vacuum expectation values (VEVs) v_i are given by

$$\phi_i = e^{i\theta_i} H_i = e^{i\theta_i} \begin{pmatrix} \frac{1}{\sqrt{2}}(v_i + R_i + iA_i) \\ h_i^- \end{pmatrix}. \quad (2)$$

The quark mass terms in the Lagrangian are

$$L_m = -\bar{U}_L [M_{u1}e^{i\theta_1} + M_{u2}e^{i\theta_2}] U_R - \bar{D}_L M_d e^{-i\theta_d} D_R + \text{h.c.}, \quad (3)$$

where $M_{ui} = -\Gamma_{ui}v_i/\sqrt{2}$.

The phases θ_1 and θ_d can be absorbed by redefining the fields U_R and D_R . However, the phase difference $\delta = \theta_2 - \theta_1$ cannot be removed, and it depends on the Higgs potential. A non-zero δ indicates spontaneous CP violation, $\delta = \delta_{\text{spon}}$. Without loss of generality, we work in the basis where D_L and D_R are already in their mass eigenstates. In this basis the down quark mass matrix M_d is diagonalized, which will be indicated by \tilde{M}_d . In general, the up quark mass matrix $M_u = M_{u1} + e^{i\delta}M_{u2}$ is not diagonal. Diagonalizing M_u produces the CKM mixing matrix. One can write $\tilde{M}_u = V_{\text{CKM}}M_uV_R^\dagger$. Here V_{CKM} is the CKM matrix and V_R is an unknown unitary matrix. A direct identification of the phase δ_{spon} with the phase δ_{KM} in the CKM matrix is not possible in general at this level. There are,

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however, classes of mass matrices that allow such a connection. A simple example is provided by setting V_R to be the unit matrix. With this condition, $M_u = V_{\text{CKM}}^\dagger \hat{M}_u$. One then needs to show that V_{CKM}^\dagger can be written as

$$V_{\text{CKM}}^\dagger = (M_{u1} + e^{i\delta} M_{u2}) \hat{M}_u^{-1}. \quad (4)$$

Expressing the CKM matrix in this form is very suggestive. If V_{CKM} (or V_{CKM}^\dagger) can always be written as a sum of two terms with a relative phase, then the phase in the CKM matrix can be identified with the phase δ .

We now demonstrate that it is the case by using the Particle Data Group (PDG) parametrization as an example. To get as close as possible to the form in (4), we write the PDG CKM matrix as [1]

$$V_{\text{CKM}} = \begin{pmatrix} e^{-i\delta_{13}} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \times \begin{pmatrix} c_{12}c_{13}e^{i\delta_{13}} & s_{12}c_{13}e^{i\delta_{13}} & s_{13} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta_{13}} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta_{13}} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta_{13}} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta_{13}} & c_{23}c_{13} \end{pmatrix}, \quad (5)$$

where $s_{ij} = \sin \theta_{ij}$ and $c_{ij} = \cos \theta_{ij}$.

Absorbing the left matrix into the definition of the U_L field, we have

$$M_{u1} = \begin{pmatrix} 0 & -s_{12}c_{23} & s_{12}s_{23} \\ 0 & c_{12}c_{23} & -c_{12}s_{23} \\ s_{13} & s_{23}c_{13} & c_{23}c_{13} \end{pmatrix} \hat{M}_u, \\ M_{u2} = \begin{pmatrix} c_{12}c_{13} & -c_{12}s_{23}s_{13} & -c_{12}c_{23}s_{13} \\ s_{12}c_{13} & -s_{12}s_{23}s_{13} & -s_{12}c_{23}s_{13} \\ 0 & 0 & 0 \end{pmatrix} \hat{M}_u, \quad (6)$$

and $\delta = -\delta_{13}$. We therefore find that it is possible to identify the CKM phase with that resulting from spontaneous CP violation. Note that as long as the phase δ is not zero, CP violation will show up in the charged currents mediated by W exchange. The effects do not disappear even when the Higgs boson masses are all set much higher than the W scale. Furthermore, $M_{1,2}$ are fixed in terms of the CKM matrix elements and the quark masses, as opposed to being arbitrary in general multi-Higgs models.

We comment that the solution is not unique, even when V_R is set to be the unit matrix. To see this, one can take another parametrization for the CKM matrix, such as the original Kobayashi–Maskawa matrix [3]. More physical requirements are needed to uniquely determine the connection. The phenomenological consequences will therefore be different. We will come back to this when we look at the phenomenology of the models. The key point we want to establish is that there are solutions in which the phase in the CKM matrix can be identified with the phase causing spontaneous CP violation in the Higgs potential.

The mass matrices M_{u1} and M_{u2} can be written in a parametrization independent way in terms of the eigen-

mass matrix \hat{M}_u , the CKM matrix, and the phase δ ,

$$M_{u1} = V_{\text{CKM}}^\dagger \hat{M}_u - \frac{e^{i\delta}}{\sin \delta} \text{Im}(V_{\text{CKM}}^\dagger) \hat{M}_u, \\ M_{u2} = \frac{1}{\sin \delta} \text{Im}(V_{\text{CKM}}^\dagger) \hat{M}_u. \quad (7)$$

Alternatively, a model can be constructed with two Higgs doublets coupled to the down sector and one Higgs doublet coupled to the up sector, so that we have

$$L_Y = \bar{Q}_L \Gamma_u \phi_u U_R + \bar{Q}_L (\Gamma_{d1} \tilde{\phi}_1 + \Gamma_{d2} \tilde{\phi}_2) D_R + \text{h.c.} \quad (8)$$

In this case $M_{di} = -\Gamma_{di} v_i / \sqrt{2}$, and

$$M_{d1} = V_{\text{CKM}} \hat{M}_d + \frac{e^{-i\delta}}{\sin \delta} \text{Im}(V_{\text{CKM}}) \hat{M}_d, \\ M_{d2} = -\frac{1}{\sin \delta} \text{Im}(V_{\text{CKM}}) \hat{M}_d. \quad (9)$$

We denote the above two possibilities as model a) with two Higgs doublets coupled to the up sector, and model b) with two Higgs doublets coupled to the down sector.

2 Model building

A common problem for models with spontaneous CP violation is that a strong QCD θ term will be generated [11]. The constraint from neutron dipole moment measurements will rule out spontaneous CP violation as the sole source if there is no mechanism to make sure that the θ term is small enough if not zero. The models mentioned above face the same problem. We therefore supplement the model with a Peccei–Quinn (PQ) symmetry [15, 16] to ensure a small θ .

To have spontaneous CP violation and also PQ symmetry simultaneously, more than two Higgs doublets are needed [17–19]. For our purpose we find that in order to have spontaneous CP violation with PQ symmetry at least three Higgs doublets $\phi_i = e^{i\theta_i} H_i$ and one complex Higgs singlet $\tilde{S} = e^{i\theta_s} S = e^{i\theta_s} (v_s + R_s + iA_s) / \sqrt{2}$ are required. The Higgs singlet with a large vacuum expectation value renders the axion from PQ symmetry breaking invisible [20–23], thus satisfying the experimental constraints on the axion couplings to fermions. We will henceforth work with models with an invisible axion [20, 21].

The PQ charges for models a) and b) are as follows

$$\text{model a)} \\ Q_L : 0, \quad U_R : -1, \quad D_R : -1, \quad \phi_{1,2} : +1, \quad \phi_d = \phi_3 : -1; \\ \text{model b)} \\ Q_L : 0, \quad U_R : +1, \quad D_R : +1, \quad \phi_{1,2} : +1, \quad \phi_u = \phi_3 : -1. \quad (10)$$

In both cases, \tilde{S} has PQ charge +2. For leptons, the PQ charges can have different assignments. For example, $L_L : 0$, $e_R : -1$ or $L_L : 0$ and $e_R : +1$.

For both model a) and b), the Higgs potentials have the form that is given by

$$\begin{aligned}
V = & -m_1^2 H_1^\dagger H_1 - m_2^2 H_2^\dagger H_2 - m_3^2 H_3^\dagger H_3 \\
& - m_{12}^2 (H_1^\dagger H_2 e^{i(\theta_2 - \theta_1)} + \text{h.c.}) - m_s^2 S^\dagger S + \lambda_1 (H_1^\dagger H_1)^2 \\
& + \lambda_2 (H_2^\dagger H_2)^2 + \lambda_t (H_3^\dagger H_3)^2 + \lambda_s (S^\dagger S)^2 \\
& + \lambda_3 (H_1^\dagger H_1)(H_2^\dagger H_2) + \lambda'_3 (H_1^\dagger H_1)(H_3^\dagger H_3) \\
& + \lambda'_3 (H_2^\dagger H_2)(H_3^\dagger H_3) + \lambda_4 (H_1^\dagger H_2)(H_2^\dagger H_1) \\
& + \lambda'_4 (H_1^\dagger H_3)(H_3^\dagger H_1) + \lambda''_4 (H_2^\dagger H_3)(H_3^\dagger H_2) \\
& + \frac{1}{2} \lambda_5 ((H_1^\dagger H_2)^2 e^{i2(\theta_2 - \theta_1)} + \text{h.c.}) \\
& + \lambda_6 (H_1^\dagger H_1)(H_1^\dagger H_2 e^{i(\theta_2 - \theta_1)} + \text{h.c.}) \\
& + \lambda_7 (H_2^\dagger H_2)(H_1^\dagger H_2 e^{i(\theta_2 - \theta_1)} + \text{h.c.}) \\
& + \lambda_8 (H_3^\dagger H_3)(H_1^\dagger H_2 e^{i(\theta_2 - \theta_1)} + \text{h.c.}) \\
& + f_1 H_1^\dagger H_1 S^\dagger S + f_2 H_2^\dagger H_2 S^\dagger S + f_3 H_3^\dagger H_3 S^\dagger S \\
& + d_{12} (H_1^\dagger H_2 e^{i(\theta_2 - \theta_1)} + H_2^\dagger H_1 e^{-i(\theta_2 - \theta_1)}) S^\dagger S \\
& + f_{13} (H_1^\dagger H_3 S e^{i(\theta_3 + \theta_s - \theta_1)} + \text{h.c.}) \\
& + f_{23} (H_2^\dagger H_3 S e^{i(\theta_3 + \theta_s - \theta_2)} + \text{h.c.}) .
\end{aligned} \tag{11}$$

Only two phases occur in the above expression, which we choose to be $\delta = \theta_2 - \theta_1$ and $\delta_s = \theta_3 + \theta_s - \theta_2$. The phase $\theta_3 + \theta_s - \theta_1$ can be written as $\delta + \delta_s$. Differentiating with respect to δ_s to get one of the conditions for minimization of the potential, we get

$$f_{13} v_1 v_3 v_s \sin(\delta_s + \delta) + f_{23} v_2 v_3 v_s \sin \delta_s = 0. \tag{12}$$

We see that δ and δ_s are related by

$$\tan \delta_s = -\frac{f_{13} v_1 \sin \delta}{f_{23} v_2 + f_{13} v_1 \cos \delta}. \tag{13}$$

Therefore, δ is the only independent phase in the Higgs potential. A non-zero $\sin \delta$ is the source of spontaneous CP violation and also the only source of CP violation in the model.

Since a large separation for the VEVs of the doublets v_i and singlet v_s is required to make the axion invisible in the model, there will be needed fine tuning between the parameters in the Higgs potential. This is a common problem for invisible axion models. We will allow such fine tuning in the model and concentrate on the implications for spontaneous CP violation and FCNC.

In this model the Goldstone fields h_w and h_z , which are "eaten" by W and Z , and the axion field are given by

$$\begin{aligned}
h_w = & \frac{1}{v} (v_1 h_1^- + v_2 h_2^- + v_3 h_3^-), \\
h_z = & \frac{1}{v} (v_1 A_1 + v_2 A_2 + v_3 A_3), \\
a = & (-v_1 v_3^2 A_1 - v_2 v_3^2 A_2 + v_{12}^2 v_3 A_3 - v^2 v_s A_s) / N_a,
\end{aligned} \tag{14}$$

where $v^2 = v_1^2 + v_2^2 + v_3^2$ and $N_a^2 = (v_{12}^2 v_3^2 v^2 + v^4 v_s^2)$ with $v_{12}^2 = v_1^2 + v_2^2$.

We remove h_w and h_z in the Yukawa interaction by making the following changes of basis:

$$\begin{aligned}
\begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_s \end{pmatrix} &= \begin{pmatrix} v_2/v_{12} & -v_1 v_3 v_s / N_A & v_1/v & -v_1 v_3^2 / N_a \\ -v_1/v_{12} & -v_2 v_3 v_s / N_A & v_2/v & -v_2 v_3^2 / N_a \\ 0 & v_{12}^2 v_s / N_A & v_3/v & v_{12}^2 v_3 / N_a \\ 0 & v_{12}^2 v_3 / N_A & 0 & -v^2 v_s / N_a \end{pmatrix} \\
&\times \begin{pmatrix} a_1 \\ a_2 \\ h_z \\ a \end{pmatrix}, \\
\begin{pmatrix} h_1^- \\ h_2^- \\ h_3^- \end{pmatrix} &= \begin{pmatrix} v_2/v_{12} & v_1 v_3 / v v_{12} & v_1/v \\ -v_1/v_{12} & v_2 v_3 / v v_{12} & v_2/v \\ 0 & -v_{12}/v & v_3/v \end{pmatrix} \begin{pmatrix} H_1^- \\ H_2^- \\ h_w \end{pmatrix}, \tag{15}
\end{aligned}$$

where $N_A^2 = v_{12}^2 (v_{12}^2 v_3^2 + v_s^2 v^2)$. $a_{1,2}$ and $H_{1,2}^-$ are the physical degrees of freedom for the Higgs fields. With the same rotation as that for the neutral pseudoscalar, the neutral scalar Higgs fields $(R_1, R_2, R_3, R_s)^T$ become $(H_1^0, H_2^0, H_3^0, H_4^0)^T$. Since the invisible axion scale v_s is much larger than the electroweak scale, to a very good approximation $N_a = v^2 v_s$ and $N_A = v_{12} v v_s$.

In the rotated basis described above, we have the Yukawa interactions for the physical Higgs degrees of freedom as follows:

$$\begin{aligned}
L_Y^{(a)} = & \bar{U}_L \left[\hat{M}_u \frac{v_1}{v_{12} v_2} - \left(\hat{M}_u - V_{\text{CKM}} \text{Im}(V_{\text{CKM}}^\dagger) \hat{M}_u \frac{e^{i\delta}}{\sin \delta} \right) \frac{v_{12}}{v_1 v_2} \right] \\
& \times U_R (H_1^0 + i a_1^0) \\
& + \bar{U}_L \hat{M}_u U_R \left[\frac{v_3}{v_{12} v} (H_2^0 + i a_2) - \frac{1}{v} H_3^0 + \frac{v_3^2}{v^2 v_s} (H_4^0 + i a) \right] \\
& - \bar{D}_L \hat{M}_d D_R \left[\frac{v_{12}}{v_3 v} (H_2^0 - i a_2) + \frac{1}{v} H_3^0 + \frac{v_{12}^2}{v^2 v_s} (H_4^0 - i a) \right] \\
& + \sqrt{2} \bar{D}_L \left[V_{\text{CKM}}^\dagger \hat{M}_u \frac{v_1}{v_2 v_{12}} \right. \\
& \left. - \left(V_{\text{CKM}}^\dagger \hat{M}_u - \text{Im}(V_{\text{CKM}}^\dagger) \hat{M}_u \frac{e^{i\delta}}{\sin \delta} \right) \frac{v_{12}}{v_1 v_2} \right] U_R H_1^- \\
& - \sqrt{2} \frac{v_3}{v_{12} v} \bar{D}_L V_{\text{CKM}}^\dagger \hat{M}_u U_R H_2^- \\
& - \sqrt{2} \frac{v_{12}}{v v_3} \bar{U}_L V_{\text{CKM}} \hat{M}_d D_R H_2^+ + \text{h.c.}, \\
L_Y^{(b)} = & \bar{D}_L \left[\hat{M}_d \frac{v_1}{v_{12} v_2} - \left(\hat{M}_d + V_{\text{CKM}}^\dagger \text{Im}(V_{\text{CKM}}) \hat{M}_d \frac{e^{-i\delta}}{\sin \delta} \right) \frac{v_{12}}{v_1 v_2} \right] \\
& \times D_R (H_1^0 - i a_1^0) \\
& + \bar{D}_L \hat{M}_d D_R \left[\frac{v_3}{v_{12} v} (H_2^0 - i a_2) - \frac{1}{v} H_3^0 + \frac{v_3^2}{v^2 v_s} (H_4^0 - i a) \right] \\
& - \bar{U}_L \hat{M}_u U_R \left[\frac{v_{12}}{v_3 v} (H_2^0 + i a_2) + \frac{1}{v} H_3^0 + \frac{v_{12}^2}{v^2 v_s} (H_4^0 + i a) \right] \\
& - \sqrt{2} \bar{U}_L \left[V_{\text{CKM}} \hat{M}_d \frac{v_1}{v_2 v_{12}} \right.
\end{aligned}$$

$$\begin{aligned}
& - \left(V_{\text{CKM}} \hat{M}_d + \text{Im}(V_{\text{CKM}}) \hat{M}_d \frac{e^{-i\delta}}{\sin \delta} \right) \frac{v_{12}}{v_1 v_2} \Big] D_R H_1^+ \\
& + \sqrt{2} \frac{v_3}{v_{12} v} \bar{U}_L V_{\text{CKM}} \hat{M}_d D_R H_2^+ \\
& + \sqrt{2} \frac{v_{12}}{v v_3} \bar{D}_L V_{\text{CKM}}^\dagger \hat{M}_u U_R H_2^- + \text{h.c.} \quad (16)
\end{aligned}$$

Note that the couplings of a and H_4^0 to the quarks are suppressed by $1/v_s$ and that only the exchange of H_1^0 and a_1^0 can induce tree level FCNC interactions. The FCNC couplings are proportional to $V_{\text{CKM}} \text{Im}(V_{\text{CKM}}^\dagger) \hat{M}_u$ and $V_{\text{CKM}}^\dagger \text{Im}(V_{\text{CKM}}) \hat{M}_d$ for models a) and b), respectively.

We have mentioned before that the identification of the phase δ with that in the CKM matrix does not uniquely determine the full Yukawa coupling. Here we give two often used parameterizations, the PDG CKM matrix and the original KM matrix with the CP violating phase indicated by δ_{KM} , to illustrate the details. In the two cases under consideration, the phases δ are identified with $-\delta_{13}$ and $-\delta_{\text{KM}}$, respectively. The differences will show up in the FCNC of the neutral Higgs coupling to quarks, which are proportional to the following quantities:

PDG :

$$\begin{aligned}
V_{\text{CKM}} \text{Im}(V_{\text{CKM}}^\dagger) \hat{M}_u &= -\sin \delta_{13} e^{i\delta_{13}} \\
&\times \begin{pmatrix} c_{13}^2 & -s_{23} s_{13} c_{13} & -c_{23} s_{13} c_{13} \\ -s_{23} s_{13} c_{13} & s_{23}^2 s_{13}^2 & s_{23} c_{23} s_{13}^2 \\ -c_{23} s_{13} c_{13} & s_{23} c_{23} s_{13}^2 & c_{23}^2 s_{13}^2 \end{pmatrix} \hat{M}_u,
\end{aligned}$$

$$\begin{aligned}
V_{\text{CKM}}^\dagger \text{Im}(V_{\text{CKM}}) \hat{M}_d &= \sin \delta_{13} e^{-i\delta_{13}} \\
&\times \begin{pmatrix} c_{12}^2 & s_{12} c_{12} & 0 \\ s_{12} c_{12} & s_{12}^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \hat{M}_d;
\end{aligned}$$

KM :

$$\begin{aligned}
V_{\text{CKM}} \text{Im}(V_{\text{CKM}}^\dagger) \hat{M}_u &= -\sin \delta_{\text{KM}} e^{i\delta_{\text{KM}}} \\
&\times \begin{pmatrix} 0 & 0 & 0 \\ 0 & s_2^2 & -s_2 c_2 \\ 0 & -s_2 c_2 & c_2^2 \end{pmatrix} \hat{M}_u,
\end{aligned}$$

$$\begin{aligned}
V_{\text{CKM}}^\dagger \text{Im}(V_{\text{CKM}}) \hat{M}_d &= \sin \delta_{\text{KM}} e^{-i\delta_{\text{KM}}} \\
&\times \begin{pmatrix} 0 & 0 & 0 \\ 0 & s_3^2 & -s_3 c_3 \\ 0 & -s_3 c_3 & c_3^2 \end{pmatrix} \hat{M}_d. \quad (17)
\end{aligned}$$

3 Meson and anti-meson mixing and neutron EDM

In this section we study some implications for meson and anti-meson mixing and the electric dipole moment of the neutron.

3.1 Meson and anti-meson mixing

Meson and anti-meson mixing has been observed previously in $K^0-\bar{K}^0$, $B_{d,s}^0-\bar{B}_{d,s}^0$ [1] and in $D^0-\bar{D}^0$ very recently [26–28]. In the models considered in the previous

section, besides the standard ‘‘box’’ diagram contributions to the mixing due to W exchange, there are also tree level contributions due to the FCNC interactions of H_1^0 and a_1 .

The interaction Lagrangian for H_l and a_k with quarks have the following form for both models a) and b):

$$L = \bar{q}_i (a_{ij}^l + b_{ij}^l \gamma_5) q_j H_l^0 + i \bar{q}_i (c_{ij}^k + d_{ij}^k \gamma_5) q_j a_k. \quad (18)$$

For the meson and anti-meson mixing, only the FCNC interaction terms of H_1^0 and a_1 contribute. We can write $a^1 = d^1 = \alpha$ and $b^1 = c^1 = \beta$, with $\alpha = (A + A^\dagger)/2$ and $\beta = (A - A^\dagger)/2$, and A given by

$$\begin{aligned}
\text{for a), } A &= V_{\text{CKM}} \text{Im}(V_{\text{CKM}}^\dagger) \hat{M}_u \frac{e^{i\delta}}{\sin \delta} \frac{v_{12}}{v_1 v_2}; \\
\text{for b), } A &= -V_{\text{CKM}}^\dagger \text{Im}(V_{\text{CKM}}) \hat{M}_d \frac{e^{-i\delta}}{\sin \delta} \frac{v_{12}}{v_1 v_2}. \quad (19)
\end{aligned}$$

Using the definition $\langle 0 | \bar{q}_i \gamma^\mu \gamma_5 q_j \rangle = i f_P p_P^\mu / \sqrt{2m_P}$ and the equation of motion $\bar{q}_i \gamma_5 q_j = (p_i - p_j)^\mu \bar{q}_i \gamma_\mu \gamma_5 q_j / (m_i + m_j)$ with $p^P = p_j - p_i$, we obtain the matrix element for $P-\bar{P}$ mixing in the vacuum saturation approximation as

$$\begin{aligned}
M_{12} &= \frac{1}{m_{H_1}^2} \left[\left(b_{ij}^2 - \frac{1}{12} (a_{ij}^2 + b_{ij}^2) \right) \frac{f_P^2 m_P^3}{(m_i + m_j)^2} \right. \\
&+ \left. \frac{1}{12} (b_{ij}^2 - a_{ij}^2) f_P^2 m_P \right] \\
&- \frac{1}{m_{a_1}^2} \left[\left(a_{ij}^2 - \frac{1}{12} (a_{ij}^2 + b_{ij}^2) \right) \frac{f_P^2 m_P^3}{(m_i + m_j)^2} \right. \\
&+ \left. \frac{1}{12} (a_{ij}^2 - b_{ij}^2) f_P^2 m_P \right] \\
&+ \frac{i 2 m_{H_1 a_1}^2}{m_{H_1}^2 m_{a_1}^2} \frac{5 a_{ij} b_{ij}}{6} \frac{f_P^2 m_P^3}{(m_i + m_j)^2}, \quad (20)
\end{aligned}$$

where $m_{H_1 a_1}^2$ parameterizes the mixing between a_1 and H_1 , which is determined from the Higgs potential $V = m_{H_1 a_1}^2 H_1 a_1 + \dots$. From the Higgs potential given earlier, we find the mixing parameters,

$$\begin{aligned}
m_{H_1 a_1}^2 &= [(\lambda_6 - \lambda_7) v_1 v_2 - \lambda_5 (v_1^2 - v_2^2) \cos \delta] \sin \delta, \\
m_{H_1 a_2}^2 &\simeq -\frac{f_{13} \sin(\delta + \delta_s) v v_s}{\sqrt{2} v_2}, \\
m_{H_2 a_1}^2 &\simeq \frac{1}{2 v_2 v} [-2 \lambda_5 v_1 v_3 v_2^2 \sin 2\delta \\
&+ 2(-\lambda_6 v_1^2 - \lambda_7 v_2^2 + (\lambda_8 + d_{12}) v_{12}^2) v_2 v_3 \sin \delta \\
&+ \sqrt{2} f_{13} v^2 v_s \sin(\delta + \delta_s)], \\
m_{H_3 a_1}^2 &= \frac{v_{12}}{v} [2 \lambda_5 v_1 v_2 \cos(\theta_1 - \theta_2) + \lambda_6 v_1^2 + \lambda_7 v_2^2 + \lambda_8 v_3^2] \\
&\times \sin \delta. \quad (21)
\end{aligned}$$

Note that all the parameters above are zero if $\sin \delta = 0$. Note also that only $m_{H_1 a_1}^2$ contribute to meson mixing, since the $H_{2,3}$ and a_2 Yukawa couplings are flavor diagonal. But the parameters $m_{H_i a_j}^2$ all contribute to the neutron EDM, which will be discussed later.

It is obvious from the structure of the flavor changing coupling in (17)) that the flavor changing structure for the PDG and KM cases are different. For the PDG case, in model a) there is a tree level contribution from neutral Higgs exchange to $D^0-\bar{D}^0$ mixing but no contribution to K^0 , B_d^0 and B_s^0 mixing. In model b), there is only a non-zero contribution to $K^0-\bar{K}^0$ mixing at the tree level. For the KM case, there is no tree level contribution to meson mixing in model a). For model b), there is only a non-zero contribution to B_s^0 mixing.

In our numerical analysis, we will use the following values for the relevant parameters. For the CKM matrix elements, we take the PDG central values with [1] $s_{12} = 0.227$, $s_{23} = 0.042$, $s_{13} = 0.004$ and $\sin \delta_{13} = 0.84$ (equivalently $s_1 = 0.227$, $s_2 = 0.0358$, $s_3 = 0.0176$ and $\sin \delta = 0.97$ for the KM parameterization). For the quark masses, we take [24] $m_u(1 \text{ GeV}) = 5 \text{ MeV}$, $m_d(1 \text{ GeV}) = 10 \text{ MeV}$, $m_s(1 \text{ GeV}) = 187 \text{ MeV}$, $m_c(m_c) = 1.30 \text{ GeV}$, $m_b(m_b) = 4.34 \text{ GeV}$ and $m_t = 174 \text{ GeV}$. For the meson decay constants, we take [25] $f_K = 156 \text{ MeV}$, $f_D = 201 \text{ MeV}$, and $f_{B_s} = 260 \text{ MeV}$.

Models with PDG parameterization

We consider the models with PDG parameterization first.

Model a): in this case there is mixing only in the $D^0-\bar{D}^0$ system. Combining the BaBar and Belle [26–28] results, the 68% C.L. range for $x = \Delta m/\Gamma_D$ is determined to be $(5.5 \pm 2.2) \times 10^{-3}$ [29–34]. Theoretically the elements in A for this particular case are $A_{12} = -s_{23}s_{13}c_{13}\frac{m_c v_{12}}{v_1 v_2}$ and $A_{21} = -s_{23}s_{13}c_{13}\frac{m_u v_{12}}{v_1 v_2}$, which implies that $a_{12} \sim b_{12} \sim -s_{23}s_{13}c_{13}\frac{m_c v_{12}}{2v_1 v_2}$. We obtain

$$\begin{aligned} x &\approx \frac{5}{12} s_{23}^2 s_{13}^2 c_{13}^2 \left(\frac{v_{12} m_c}{v_1 v_2} \right)^2 \frac{f_D^2 m_D}{\Gamma_D} \left(\frac{m_D}{m_c + m_u} \right)^2 \\ &\times \left(\frac{1}{m_{H_1}^2} - \frac{1}{m_{a_1}^2} \right) \\ &= 7.5 \times 10^{-5} \frac{1}{(\sin 2\beta)^2 v_{12}^2} \left(\frac{1}{m_{H_1}^2} - \frac{1}{m_{a_1}^2} \right) (100 \text{ GeV})^4, \end{aligned} \quad (22)$$

where $\tan \beta$ is defined to be v_1/v_2 .

It is well known that the SM short distance contribution to the $D-\bar{D}$ mixing is small. Long distance contributions can be much larger, but they suffer from considerable uncertainty. New physics may contribute significantly [29–34]. It is tempting to see if the new contribution in this model can account for the full measured value. If the effective neutral Higgs mass $m_{\text{eff}}^2 = 1/(1/m_{H_1}^2 - 1/m_{a_1}^2)$ is of order 100 GeV, one would require $\sin^2 2\beta v_{12}^2 \sim (12)^2 \text{ GeV}^2$. Since $v_{1,2}$ are related to the top quark mass, with the assumption that the top quark Yukawa coupling $y_t \leq 1$, one of them should be large, $\sim 240 \text{ GeV}$. Saturating the experimental central value for x , we would have $\sin(2\beta) \sim 0.05$ implying v_1/v_2 or v_2/v_1 to be of the order of 1/40. If all VEVs are of the same order of magnitude, the new contribution does not produce a large enough x to saturate the measured value.

Model b): in this case there is mixing only in the $K^0-\bar{K}^0$ system. We have

$$\frac{\Delta m_K}{m_K} = 4.4 \times 10^{-12} \frac{1}{\sin^2 2\beta v_{12}^2} \left(\frac{1}{m_{H_1}^2} - \frac{1}{m_{a_1}^2} \right) (100 \text{ GeV})^4. \quad (23)$$

This is to be compared with the experimental data, $\Delta m_K/m_K = 7.0 \times 10^{-15}$. It puts strong constraints on the scalar masses, i.e., the Higgs particles must be at least in the TeV scale to suppress the value if a_1 and H_1 are not degenerate in mass.

In this model there is also a contribution to the CP violating parameter ϵ for $K^0-\bar{K}^0$ at the tree level if $m_{H_1 a_1}^2$ is not zero, which is true in general. Using (20), we find that the H_1 and a_1 contributions to M_{12} have the following relation:

$$\frac{\text{Im}(M_{12})}{\text{Re}(M_{12})} = \frac{2m_{H_1 a_1}^2}{m_{H_1}^2 - m_{a_1}^2}. \quad (24)$$

Combining information from the above relation, the experimental value of $|\epsilon| = (2.233 \pm 0.015) \times 10^{-3}$, and the constraint from Δm_K discussed above, we find that $|2m_{H_1 a_1}^2/(m_{H_1}^2 - m_{a_1}^2)|$ is constrained to be less than 6×10^{-3} .

Models with KM parameterization

We now come to models with the original KM parameterization. In this case, there is no meson and anti-meson mixing in model a).

Model b): there is mixing only in the $B_s-\bar{B}_s$ system. We have

$$\frac{\Delta m_{B_s}}{m_{B_s}} = 9.5 \times 10^{-12} \frac{1}{\sin^2 2\beta v_{12}^2} \left(\frac{1}{m_{H_1}^2} - \frac{1}{m_{a_1}^2} \right) (100 \text{ GeV})^4. \quad (25)$$

The experimental value $\Delta m_{B_s} = 17.4 \text{ ps}^{-1}$ implies $\Delta m_{B_s}/m_{B_s} = 2.1 \times 10^{-12}$. It has been shown in [35–37] that the new physics contribution to Δm_{B_s} can be up to 10%. To obtain the lowest Higgs boson mass, we maximize $\sin 2\beta = 1$, which requires $v_1 = v_2$. Taking $v_{1,2,3}$ to be all equal, the Higgs boson mass can be as low as 300 GeV. Smaller $v_{1,2}$ or non-equal v_1 and v_2 would lead to more stringent bound on the Higgs mass.

3.2 The neutron EDM

The neutron EDM can also provide much information on the model parameters. The standard model predicts a very small [38–41] $d_n (< 10^{-31} e \text{ cm})$. The present experimental upper bound on the neutron EDM d_n is very tight [1]: $|d_n| < 0.63 \times 10^{-25} e \text{ cm}$. We now study whether the neutron EDM can reach its present bound after imposing the constraints from meson and anti-meson mixing discussed in the previous section.

In the models we are studying, the quark EDMs will be generated at loop levels due to mixing between a_i and H_i . The one loop contributions to the neutron EDM are suppressed for the usual reason of being proportional to light quarks masses to the third power for a diagram in which the internal quark is the same as the external quark. In model a) with PDG parameterization, there is a potentially large contribution when there is a top quark in the loop. However, the couplings to the top are proportional to s_{13} ; therefore, the contribution to the neutron EDM is much smaller than the present upper bound. We will not discuss them further.

It is well known that exchange of Higgs at the two loop level may be more important than the one loop contribution, through the quark EDM O_q^γ [42–44], quark color EDM O_q^C [42–44], and the gluon color EDM O_g^C [45, 46] defined as

$$\begin{aligned} O_q^\gamma &= -\frac{d_q}{2} i\bar{q}\sigma_{\mu\nu}\gamma_5 F^{\mu\nu}q, & O_q^C &= -\frac{f_q}{2} ig_s\bar{q}\sigma_{\mu\nu}\gamma_5 G^{\mu\nu}q, \\ O_g^C &= -\frac{1}{6} C f_{abc} G_{\mu\nu}^a G_{\mu\alpha}^b \tilde{G}_{\nu\alpha}^c, \end{aligned} \quad (26)$$

where $F^{\mu\nu}$ is the photon field strength, $G^{\mu\nu}$ is the gluon field strength and $\tilde{G}^{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\alpha\beta}G^{\alpha\beta}$.

In the valence quark model, the quark EDM and color EDM contributions to the neutron EDM d_n are given by [38–41]

$$d_n^\gamma = \eta_d \left[\frac{4}{3}d_d - \frac{1}{3}d_u \right]_\Lambda, \quad d_n^C = e\eta_f \left[\frac{4}{9}f_d + \frac{2}{9}f_u \right]_\Lambda, \quad (27)$$

where [47, 48] $\eta_d = \left(\frac{\alpha_s(M_Z)}{\alpha_s(m_b)}\right)^{16/23} \left(\frac{\alpha_s(m_b)}{\alpha_s(m_c)}\right)^{16/25} \left(\frac{\alpha_s(m_c)}{\alpha_s(\Lambda)}\right)^{16/27} \approx 0.166$ and $\eta_f = \left(\frac{\alpha_s(M_Z)}{\alpha_s(m_b)}\right)^{14/23} \left(\frac{\alpha_s(m_b)}{\alpha_s(m_c)}\right)^{14/25} \left(\frac{\alpha_s(m_c)}{\alpha_s(\Lambda)}\right)^{14/27} \frac{\alpha_s(M_Z)}{\alpha_s(\Lambda)} \approx 0.0117$ are the QCD running factors from the scale m_Z to the hadron scale Λ .

A naive dimensional analysis (NDA) estimate gives the gluon color EDM contribution to the neutron EDM as follows:

$$d_n \approx \frac{eM}{4\pi} \xi C, \quad (28)$$

where $M = 4\pi f_\pi = 1190$ MeV is the scale of the chiral symmetry breaking. The QCD running factor is [49, 50] $\xi = \left(\frac{g(\Lambda)}{4\pi}\right)^3 \left(\frac{\alpha_s(m_b)}{\alpha_s(m_t)}\right)^{-54/23} \left(\frac{\alpha_s(m_c)}{\alpha_s(m_b)}\right)^{-54/25} \left(\frac{\alpha_s(\Lambda)}{\alpha_s(m_c)}\right)^{-54/27} \approx 1.2 \times 10^{-4}$.

The two loop contributions d_q , f_q and C are given by

$$\begin{aligned} d_q &= \frac{e\alpha_{em}Q_q}{24\pi^3} m_q G(q), & f_q &= \frac{\alpha_s}{64\pi^3} m_q G(q), \\ C &= \frac{1}{8\pi} H(g), \end{aligned} \quad (29)$$

where Q_q is the charge of q quark and

$$\begin{aligned} G(q) &= \left[\left(f \left(\frac{m_t^2}{m_{H_1}^2} \right) - f \left(\frac{m_t^2}{m_{a_k}^2} \right) \right) \text{Im} Z_{tq}^{lk} \right. \\ &\quad \left. + \left(g \left(\frac{m_t^2}{m_{H_1}^2} \right) - g \left(\frac{m_t^2}{m_{a_k}^2} \right) \right) \text{Im} Z_{qt}^{lk} \right], \\ H(g) &= \left(h \left(\frac{m_t^2}{m_{H_1}^2} \right) - h \left(\frac{m_t^2}{m_{a_k}^2} \right) \right) \text{Im} Z_{tt}^{lk}, \end{aligned} \quad (30)$$

where $\text{Im} Z_{ij}$ is defined through $\text{Im} Z_{ij}^{lk} = 2a_{ii}^l d_{jj}^k \lambda_{lk} / (m_i m_j)$ with a^l and d^k defined by (18), and $\lambda_{lk} = m_{H_1 a_k}^2 / (m_{H_1}^2 - m_{a_k}^2)$ is a mixing factor depending on the neutral Higgs bosons exchanged in the loop.

The functions $f(z)$, $g(z)$ and $h(z)$ are given by

$$\begin{aligned} f(z) &= \frac{z}{2} \int_0^1 dx \frac{1-2x(1-x)}{x(1-x)-z} \ln \frac{x(1-x)}{z}, \\ g(z) &= \frac{z}{2} \int_0^1 dx \frac{1}{x(1-x)-z} \ln \frac{x(1-x)}{z}, \\ h(z) &= \frac{z^2}{2} \int_0^1 dx \int_0^1 du \frac{u^3 x^3 (1-x)}{[zx(1-ux) + (1-u)(1-x)]^2}. \end{aligned} \quad (31)$$

Numerically we find that the functions (f, g, h) change slowly from $(0.5, 1, 0.1)$ to $(0.2, 0.2, 0.03)$ when the Higgs masses are increased from 100 GeV to 1 TeV.

Models with PDG parameterization

Model a): the two loop contributions to the neutron EDM due to the Higgs bosons exchange in the loop are proportional to the mixing factor $\lambda_{lk}(f, g, h)$. We take these factors to be approximately equal to estimate the contributions from different Higgs exchanges.

If using the parameters that produce D mixing, i.e., $\tan\beta = 40$, $v_{12} \sim 240$ GeV and $v_3 \sim 10$ GeV and a Higgs value around 100 GeV are used, we find that the dominant contribution is from H_3, a_1 exchange,

$$d_n \approx -1.5 \times 10^{-25} \frac{m_{H_3 a_1}^2}{m_{H_3}^2 - m_{a_1}^2} e \text{ cm}. \quad (33)$$

If all VEVs are of the same order, i.e., taking $v_1 = v_2 = v_3$ with a Higgs mass of order 100 GeV, we have

$$d_n \approx 8 \times 10^{-26} \frac{m_{H_3 a_1}^2}{m_{H_3}^2 - m_{a_1}^2} e \text{ cm}. \quad (34)$$

Model b): in this case H_1 and a_1 do not couple to $\bar{t}t$, so the two loop contribution to the quark EDM and the quark and gluon color EDM from the H_1 and a_1 are small.

The contributions to the neutron EDM are about the same from the H_1, a_2 and $H_{2,3}, a_1$ exchange, with different mixing factors. Explicitly as an example, for the case H_1 and a_2 exchange with the Higgs mass taken to be 1 TeV, as high as allowed by $K^0 - \bar{K}^0$ mixing, we have

$$d_n \approx -1 \times 10^{-26} \frac{m_{H_1 a_2}^2}{m_{H_1}^2 - m_{a_2}^2} e \text{ cm}. \quad (35)$$

If $m_{H_1 a_2}^2$ is not too much smaller than m_{H_1, a_2}^2 , the neutron EDM can be close to the upper bound. The contribution from H_1 and a_1 mixing is smaller due to the constraints from ϵ discussed earlier.

Models with KM parameterization

Model a): in this case there are no constraints from meson mixing, and the Higgs mass can be low. If all VEVs are of the same order, i.e. taking $v_1 = v_2 = v_3$ with Higgs mass of order 100 GeV, we have the main contribution coming from H_1, a_2 exchange,

$$d_n \approx 5 \times 10^{-26} \frac{m_{H_1 a_2}^2}{m_{H_1}^2 - m_{a_2}^2} e \text{ cm}. \quad (36)$$

Model b): similar to the case for model b) as in the PDG parameterization case, the contributions from the H_1 and a_1 exchange are small. Taking the VEVs to be of the same order and the Higgs mass to be of the order of 100 GeV, we find that the contributions from H_1, a_2 exchange and $H_{2,3}, a_1$ exchange are comparable. For the case of H_1 and a_2 exchange, the contribution is given by

$$d_n \approx 5 \times 10^{-26} \frac{m_{H_1 a_2}^2}{m_{H_1}^2 - m_{a_2}^2} e \text{ cm}. \quad (37)$$

If one takes the Higgs mass to be 300 GeV as that from $B_s - \bar{B}_s$ mixing, the neutron EDM will be smaller.

4 Discussion and conclusions

In our previous discussions, we have not considered Yukawa coupling for the lepton sector. An analogous study can be carried out. If one introduces right-handed neutrinos, the see-saw mechanism can be applied to generate small neutrino masses if the axion scale v_s is identified with the see-saw scale. We briefly discuss two classes of models parallel to the quark sector before our conclusion.

Model a): the PQ charges for the lepton doublet L_L , the electron e_R and neutrino ν_R are assigned as follows: $L_L(0)$, $e_R(-1)$ and $\nu_R(-1)$. The Yukawa couplings are then

$$L = \bar{L}_L (Y_1 H_1 + Y_2 H_2 e^{i\delta}) \nu_R + \bar{L}_L Y_3 \tilde{H}_3 e_R + \bar{\nu}_R^C Y_s S e^{i(\delta+\delta_s)} \nu_R + \text{h.c.} \quad (38)$$

In this case the mass matrices in $L_m = -\bar{e}_L M_e e_R - \bar{\nu}_L M_D \nu_R - (1/2) \bar{\nu}_R^C M_R \nu_R$ can be written as

$$M_l = -\frac{1}{\sqrt{2}} Y_3 v_3, \quad M_D = -\frac{1}{\sqrt{2}} (Y_1 v_1 + Y_2 v_2 e^{i\delta}), \\ M_R = -\sqrt{2} Y_s v_s e^{i(\delta+\delta_s)}. \quad (39)$$

The charged current mixing matrix in the lepton sector, the Pontecove–Maki–Nakagawa–Sakata (PMNS) matrix [51, 52], V_{PMNS} , similar to the V_{CKM} matrix is given by $V_{\text{PMNS}} = V_L^e V_L^{\nu\dagger}$, where V_L^e and V_L^{ν} are defined by $M_e =$

$V_L^{e\dagger} \hat{M}_e V_R^e$ and $M_\nu = -M_D M_R^{-1} M_D^T = V_L^{\nu\dagger} \hat{M}_\nu V_L^{\nu*}$ with \hat{M}_e and \hat{M}_ν the charged lepton and light neutrino eigen-mass matrices.

Model b): the PQ charges for the lepton doublet L_L , the electron e_R and neutrino ν_R are assigned as follows: $L_L(0)$, $e_R(+1)$ and $\nu_R(+1)$. The Yukawa couplings are

$$L = \bar{L}_L Y_3 H_3 \nu_R + \bar{L}_L (Y_1 \tilde{H}_1 + Y_2 \tilde{H}_2 e^{-i\delta}) e_R + \bar{\nu}_R^C Y_s S^\dagger e^{-i(\delta+\delta_s)} \nu_R + \text{h.c.}, \quad (40)$$

and

$$M_l = -\frac{1}{\sqrt{2}} (Y_1 v_1 + Y_2 v_2 e^{-i\delta}), \quad M_D = -\frac{1}{\sqrt{2}} Y_3 v_3, \\ M_R = -\sqrt{2} Y_s v_s e^{-i(\delta+\delta_s)}. \quad (41)$$

From the above we see that, in general, there is CP violation in the mixing matrix V_{PMNS} , and the source is the same as that in the Higgs potential. But the identification of the phase δ with the phase in the V_{PMNS} becomes more complicated due to the appearance of M_R . The related details will be discussed elsewhere.

We have proposed that the CP violating phase in the CKM mixing matrix be the same as that causing spontaneous CP violation in the Higgs potential. Specific multi-Higgs doublet models have been constructed to realize this idea. There are flavor changing neutral currents mediated by neutral Higgs bosons at the tree level. However, even when the Higgs boson masses are set to be very large, the phase in the CKM matrix can be made finite and CP violating effects will not disappear, unlike in other models of spontaneous CP violation where the CP violation disappears when the Higgs boson masses become large. Another interesting feature of this model is that the FCNC Yukawa couplings are fixed in terms of the quark masses and CKM mixing angles, making a phenomenological analysis much easier.

We have studied some implications for meson–anti-meson mixing, including recent data on $D - \bar{D}$ mixing, and the electric dipole moment of the neutron. We find that the neutral Higgs boson masses can be at the order of 100 GeV. The neutron EDM can be close to the present experimental upper bound.

Acknowledgements. This work was supported in part by the National Science Council and the National Center for Theoretical Sciences, and by the U.S. Department of Energy under Grants No. DE-FG02-96ER40969. We thank Jon Parry for pointing out a typo in our first version on the arXiv.

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