Model for particle masses, flavor mixing, and *CP* violation, based on spontaneously broken discrete chiral symmetry as the origin of families

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We construct extensions of the standard model based on the hypothesis that Higgs bosons also exhibit a family structure and that the flavor weak eigenstates in the three families are distinguished by a discrete Z_6 chiral symmetry that is spontaneously broken by the Higgs sector. We study in detail at the tree level models with three Higgs doublets and with six Higgs doublets comprising two weakly coupled sets of three. In a leading approximation of S_3 cyclic permutation symmetry the three-Higgs-doublet model gives a ''democratic'' mass matrix of rank 1, while the six-Higgs-doublet model gives either a rank-1 mass matrix or, in the case when it spontaneously violates *CP*, a rank-2 mass matrix corresponding to nonzero second family masses. In both models, the CKM matrix is exactly unity in the leading approximation. Allowing small explicit violations of cyclic permutation symmetry generates small first family masses in the six-Higgs-doublet model, and first and second family masses in the three-Higgs-doublet model, and gives a nontrivial CKM matrix in which the mixings of the first and second family quarks are naturally larger than mixings involving the third family. Complete numerical fits are given for both models, flavor-changing neutral current constraints are discussed in detail, and the issues of unification of couplings and neutrino masses are addressed. On a technical level, our analysis uses the theory of circulant and retrocirculant matrices, the relevant parts of which are reviewed. [S0556-2821(98)01523-9]

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I. INTRODUCTION

It has long been recognized that the hierarchical structures of the family mass spectra, with their large third family masses, and of the Cabibbo-Kobayashi-Maskawa (CKM) mixing matrix, with its suppressed third family mixings, may have a common dynamical origin. In particular, several authors [1] have stressed that the observed pattern seems to be close to the ''rank-1'' limit, in which the mass matrices have the ''democratic'' form of a matrix with all matrix elements equal to unity, which has one eigenvalue 3 and two eigenvalues 0; when both up and down quark mass matrices have this form, they are diagonalized by the same unitary transformation and the CKM matrix is unity. A generalization of the democratic form, which is closely related to the models developed below, is the suggestion of Harrison and Scott [2] that the Hermitian square of the mass matrix should have the form of a circulant matrix. Because the underlying dynamical basis for these choices has not been apparent, it has not been possible to systematically extend them to renormalizable field theory models that incorporate, and relate, the observed mass and mixing hierarchies.

We present in this paper models for the quark mass and flavor mixing matrices, based on the underlying dynamical assumption that the three-flavor weak eigenstates are distinguished by different eigenvalues of a discrete chiral Z_6 quantum number. The idea that a discrete chiral quantum number may underlie family structure was introduced originally by Harari and Seiberg [3], and was developed recently by the author [4] in a modified form that we follow here. Also of relevance is the remark of Weinberg [5] that an unbroken discrete chiral quantum number suffices to enforce the masslessness of fermionic states. Extending the general framework of this earlier work, we postulate that all *complex* fields carry a discrete chiral family quantum number. Since the Higgs scalars in the standard model are complex, we introduce one or two triplets of Higgs doublets that carry Z_6 quantum numbers, and that are coupled to the fermions by Yukawa couplings constructed so that the Lagrangian is exactly Z_6 invariant. Spontaneous symmetry breaking, in which the neutral members of the three or six Higgs doublets acquire vacuum expectations, then gives the fermion mass matrices that form the basis for our detailed analysis.

In addition to postulating that the Lagrangian has an exact discrete chiral symmetry that is spontaneously broken, we also postulate that there is an S_3 cyclic symmetry under cyclic permutation of the flavor eigenstates that is explicitly but weakly broken by the Yukawa couplings and the Higgs self-couplings in the Lagrangian. This assumption permits the analysis of our models by developing them in a perturbation expansion in powers of the S_3 cyclic symmetry breaking, leading, as we shall see, to qualitative features of the mass and mixing hierarchies that accord with observation. An interplay of spontaneously broken symmetries with weakly explicitly broken symmetries has played a useful role in particle phenomenology in the past, most notably in understanding the consequences of chiral symmetry in quantum chromodynamics. Our analysis suggests that such an interplay, in the context of electroweak symmetry breaking, may also provide a basis for understanding features of the mass and mixing hierarchy.

This paper is organized as follows. In Sec. II we elaborate on the form of and motivation for our basic assumptions of

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an exact discrete chiral symmetry and an approximate S_3 cyclic permutation symmetry. In Sec. III we write down the Lagrangians for two extensions of the standard model that incorporate these assumptions, the first based on a single three-family set of Higgs doublets and the second based on including an additional weakly coupled three-family set of Higgs doublets. In Sec. IV we review the theory of circulant and retrocirculant matrices, in the framework of the 3×3 matrices that are needed for the subsequent analysis. In Sec. V we discuss the extrema of the Higgs potentials in the three- and six-doublet models, in the limit of exact S_3 cyclic symmetry. We work out the spectra of physical Higgs particles, and show that for a wide range of parameters, the six-doublet model leads to spontaneous violation of *CP*. In a related appendix, Appendix A, we give the formulas needed for numerical minimization of the Higgs potentials by the conjugate gradient method. In Sec. VI we use the extrema determined in Sec. V to calculate the tree approximation mass matrices. We show that in the limit of exact cyclic permutation symmetry, the mass matrices are retrocirculants, corresponding to the rank-1 ''democratic'' form in the three-doublet model and to a rank-2 generalization in the six-doublet model when *CP* is spontaneously violated. Also, in the limit of exact cyclic permutation symmetry, we characterize the Higgs decay modes, and show that the CKM matrix is exactly unity and that strangeness-changing neutral currents exactly vanish. In Sec. VII we formulate a perturbative expansion around the zeroth order approximation of exact S_3 cyclic permutation symmetry, and show that the mixing matrix for the first and second families is zeroth order in the perturbation, whereas the mixings involving the third family are first order in the perturbation. In Sec. VIII we derive formulas for the contributions from Higgs exchange to the K_L-K_S mass difference, which is the process most sensitive to strangeness-changing neutral current effects. In Sec. IX we describe the procedure used for making overall fits of our model, including small violations of cyclic permutation symmetry, to the data, give sample numerical results, and draw some conclusions from these. In Sec. X we summarize experimental signatures for our model, comment on its extension to neutrino masses and mixings, discuss the prospects for coupling constant unification, and give some directions for future investigations.

II. BASIC ASSUMPTIONS: AN EXACT DISCRETE CHIRAL SYMMETRY AND AN APPROXIMATE S_3 CYCLIC SYMMETRY

In formulating our basic assumptions, we shall follow a procedure that has worked well in the past as a heuristic tool in particle physics. This is to abstract symmetry or partial symmetry assumptions from specific simplified field theory models, and then to discard the models, but to retain the symmetry assumptions deduced from them as the basis for phenomenological calculations. Examples where this has been a productive method in the past include (1) the CVC (conserved vector current) and PCAC (partially conserved axial vector current) symmetries of the strong interactions, the algebra of currents, and the calculational methods based on these, and (2) the approximate SU(3) flavor symmetry of the strong interactions. These postulates, which had a somewhat *ad hoc* character at the time when they were first introduced, helped pave the way for the formulation of the standard model, into which they were incorporated in a natural way and thereby ultimately justified.

Our aim in this paper is to apply a similar method to the problems of family structure and mass and mixing matrices, which to date have been among the most vexing puzzles of the standard model. As a heuristic field theoretic model, we shall adopt a simplified composite model in which all matter particles (quarks, leptons, and Higgs fields — everything other than the gauge fields) are composites of a single fermion field χ. As observed by Harari and Seiberg [3] and Weinberg [5], in a gauge theory for χ the instanton determinant that breaks global U(1) invariance leaves unbroken a discrete Z_{2K} chiral subgroup, with K determined by the index of the representation of the gauge group under which χ transforms. Harari and Seiberg propose, moreover, that this naturally occurring discrete chiral subgroup provides the quantum number that distinguishes between the various families. Since it is now clear that there are exactly three light families, we shall assume henceforth in applying this idea that $K=3$, so that we start from the assumption that the fundamental Lagrangian, as augmented by the instanton-induced potential, is invariant under the simultaneous transformations

$$\chi_L\rightarrow\chi_L\exp(2\pi i/6),\quad \chi_R\rightarrow\chi_R\exp(-2\pi i/6) \tag{1a}$$

of the fundamental fermion fields χ. The fields in the low energy effective Lagrangian are in general nonlinear functionals of the fundamental fields. Fermionic effective fields must be odd monomials in the fundamental fields, and so can come in three varieties ψ_n with the discrete chiral transformation law

$$\begin{aligned}&\psi_{nL}\rightarrow\psi_{nL}\exp[(2n+1)2\pi i/6],\\ &\psi_{nR}\rightarrow\psi_{nR}\exp[-(2n+1)2\pi i/6],\quad n=1,2,3,\end{aligned} \tag{1b}$$

while complex bosonic effective fields must be even monomials in the fundamental fermion fields, and so can also come in three varieties ϕ_n with the discrete chiral transformation law

$$\phi_n\rightarrow\phi_n\exp(2n2\pi i/6),\quad n=1,2,3. \tag{1c}$$

Introducing the cube roots of unity ω and $\overline{\omega}$,

$$\omega=\exp(2\pi i/3)=-\frac{1}{2}+\frac{\sqrt{3}}{2}i,$$

$$\overline{\omega}=\exp(-2\pi i/3)=-\frac{1}{2}-\frac{\sqrt{3}}{2}i, \tag{2a}$$

which obey the relations

$$\overline{\omega}=\omega^*=\omega^2,\quad 1+\omega+\overline{\omega}=0, \tag{2b}$$

the transformation laws of Eqs. (1a)–(1c) take the form

$$\chi_L \to \chi_L \omega^{1/2}, \quad \chi_R \to \chi_R \overline{\omega}^{1/2},$$
$$\psi_{nL} \to \psi_{nL} \omega^{n+1/2}, \quad \psi_{nR} \to \psi_{nR} \overline{\omega}^{n+1/2}, \quad n=1,2,3, \tag{3}$$
$$\phi_n \to \phi_n \omega^n, \quad n=1,2,3.$$

Gauge fields are real fields, and since the phase in Eq. (1c) never takes the value -1 for any n, the gauge fields in a Z_6 model necessarily come in only one variety, transforming with phase unity under discrete chiral transformations. Thus the minimal Z_6-invariant extension of the standard model consists of a triplicated set of fermions and a triplicated set of Higgs doublets, obeying the transformation laws of Eqs. (1b) and (1c), respectively, together with the usual gauge bosons, with the Lagrangian constructed to be Z_6 invariant.

As we shall see in Sec. III below, the assumption of an unbroken discrete chiral symmetry still leaves many parameters in the Lagrangian, and it is desirable to look for a further exact or approximate symmetry to impose. The natural candidate is S_3 cyclic permutation symmetry, under simultaneous cyclic permutation of the $n=1,2,3$ discrete chiral components of the fermion and Higgs boson fields. If the discrete chiral components were physically identical, one would expect this S_3 cyclic symmetry to be exact. However, in the composite picture from which we are abstracting our model, the discrete chiral components differ physically by the addition of fermion-antifermion pairs coupled as Lorentz scalars, and so the internal wave functions of the discrete chiral components are different. Thus the best we might hope for is an approximate, weakly broken, S_3 cyclic permutation symmetry, and this will be assumed as the second ingredient of our model.

By abstracting our two fundamental assumptions from a schematic composite model, we gain some assurance that they are consistent with each other and at least physically plausible. However, we do not attach great significance to the particular model from which they were inferred; it is entirely possible that the same assumptions can emerge from other dynamical frameworks. We shall henceforth avoid further discussion of underlying models, and focus on exploring the consequences of our assumptions within the standard framework of low energy renormalizable effective action phenomenology.

III. DISCRETE-CHIRAL-INVARIANT EXTENSIONS OF THE STANDARD MODEL

We proceed now to write down discrete-chiral-invariant extensions of the Lagrangian density for the standard model, following the notation of the text of Mohapatra [6]. In the following, each quark or lepton field is implicitly a column vector formed from the three discrete chiral components obeying the transformation laws of Eq. (3), with the $n=1$ index at the top of the column vector and the $n=3$ index at the bottom. For the Higgs scalar fields, the discrete chiral subscript n will be indicated explicitly. We shall be interested in two models, the first containing a single discrete chiral triplet of Higgs doublets ϕ, the second containing two discrete chiral triplets of Higgs doublets, denoted, respectively, by ϕ and η. We shall write all formulas for the case of the six-Higgs-doublet model; the simpler three-doublet model is obtained by setting all fields η to zero.

The total Lagrangian density $\mathcal{L}$ consists of kinetic terms for the gauge, Higgs, and fermionic fields, together with Yukawa couplings of the Higgs fields to the fermions and the Higgs self-interaction potential. Writing

$$\mathcal{L}=\mathcal{L}_{\text{gauge kinetic}}+\mathcal{L}_{\text{Higgs kinetic}}+\mathcal{L}_{\text{fermion kinetic}} +\mathcal{L}_{\text{Yukawa}}+\mathcal{L}_{\text{Higgs potential}}, \tag{4a}$$

the gauge kinetic terms have the usual form

$$\mathcal{L}_{\text{gauge kinetic}}=-\tfrac{1}{4}\vec{W}_{\mu\nu}\cdot\vec{W}_{\mu\nu}-\tfrac{1}{4}B_{\mu\nu}B_{\mu\nu},$$
$$\vec{W}_{\mu\nu}=\partial_\mu\vec{W}_\nu-\partial_\nu\vec{W}_\mu+g\vec{W}_\mu\times\vec{W}_\nu,$$
$$B_{\mu\nu}=\partial_\mu B_\nu-\partial_\nu B_\mu, \tag{4b}$$

and so also do the fermion kinetic terms (with Q_L and ψ_L, respectively, the left-handed quark and lepton doublets, and $\vec{\tau}$ the weak isospin Pauli matrices that act on them):

$$\begin{aligned}\mathcal{L}_{\text{fermion kinetic}} &=-\overline{Q}_L\gamma_\mu\left(\partial_\mu-\frac{ig}{2}\vec{\tau}\cdot\vec{W}_\mu-\frac{ig'}{6}B_\mu\right)Q_L\\ &\quad-\overline{\psi}_L\gamma_\mu\left(\partial_\mu-\frac{ig}{2}\vec{\tau}\cdot\vec{W}_\mu+\frac{ig'}{6}B_\mu\right)\psi_L\\ &\quad-\overline{e}_R\gamma_\mu(\partial_\mu+ig'B_\mu)e_R-\overline{\nu}_R\gamma_\mu\partial_\mu\nu_R\\ &\quad-\overline{u}_R\gamma_\mu\left(\partial_\mu-\frac{2ig'}{3}B_\mu\right)u_R-\overline{d}_R\gamma_\mu\left(\partial_\mu+\frac{ig'}{3}B_\mu\right)d_R.\end{aligned} \tag{4c}$$

The Higgs kinetic energy is simply a sum over kinetic terms of the standard form for the discrete chiral components of the scalars ϕ and η (each of which is, as usual, a weak isospin doublet):

$$\begin{aligned}\mathcal{L}_{\text{Higgs kinetic}}=&-\sum_{n=1,2,3}\left|\partial_\mu\phi_n-\frac{ig}{2}\vec{\tau}\cdot\vec{W}_\mu\phi_n-\frac{ig'}{2}B_\mu\phi_n\right|^2\\ &-\sum_{n=1,2,3}\left|\partial_\mu\eta_n-\frac{ig}{2}\vec{\tau}\cdot\vec{W}_\mu\eta_n-\frac{ig'}{2}B_\mu\eta_n\right|^2.\end{aligned} \tag{4d}$$

It is only in the Yukawa couplings and the Higgs potential that invariance under discrete chiral transformations plays a nontrivial role. Letting $\tilde{\phi}_n$ and $\tilde{\eta}_n$ denote the CP conjugates of the Higgs fields,

$$\tilde{\phi}_n=(CP)^{-1}\phi_n CP=i\tau_2\phi_n^*,$$
$$\tilde{\eta}_n=(CP)^{-1}\eta_n CP=i\tau_2\eta_n^*, \tag{5a}$$

the Yukawa Lagrangian takes the form

$$\mathcal{L}_{\text{Yukawa}}=\overline{Q_L}\Phi^d d_R+\overline{Q_L}\Phi^u u_R + \overline{\psi_L}\Phi^e e_R+\overline{\psi_L}\Phi^\nu \nu_R+\text{adjoint}, \tag{5b}$$

where Φ^f, $f=d,u,e,\nu$ is a 3×3 matrix acting on the discrete chiral column vector structure, and where we have allowed for the possibility of nonzero Dirac neutrino masses by including a right-handed neutrino. The matrices Φ^f must be constructed so that Eq. (5b) is invariant under simultaneous discrete chiral transformations of the fermion and Higgs fields. Referring to Eq. (3), it is easy to see that this dictates the structure

$$\Phi^f=g_\phi^f(P_{\phi1}^f\phi_1+P_{\phi2}^f\phi_2+P_{\phi3}^f\phi_3) + g_\eta^f(P_{\eta1}^f\eta_1+P_{\eta2}^f\eta_2+P_{\eta3}^f\eta_3), \quad f=d,e,$$
$$\Phi^f=g_\phi^f(P_{\phi1}^f\tilde{\phi}_2+P_{\phi2}^f\tilde{\phi}_1+P_{\phi3}^f\tilde{\phi}_3) + g_\eta^f(P_{\eta1}^f\tilde{\eta}_2+P_{\eta2}^f\tilde{\eta}_1+P_{\eta3}^f\tilde{\eta}_3), \quad f=u,\nu, \tag{6a}$$

with the 3×3 matrices $P_{\xi n}^f$ given, for all flavors $f=u,d,e,\nu$ and for $\xi=\phi,\eta$, by

$$P_{\xi1}^f=\begin{pmatrix}0 & 1+\beta_{\xi12}^f & 0\\ 1+\beta_{\xi21}^f & 0 & 0\\ 0 & 0 & 1+\beta_{\xi33}^f\end{pmatrix},$$
$$P_{\xi2}^f=\begin{pmatrix}0 & 0 & 1+\beta_{\xi13}^f\\ 0 & 1+\beta_{\xi22}^f & 0\\ 1+\beta_{\xi31}^f & 0 & 0\end{pmatrix}, \tag{6b}$$
$$P_{\xi3}^f=\begin{pmatrix}1+\beta_{\xi11}^f & 0 & 0\\ 0 & 0 & 1+\beta_{\xi23}^f\\ 0 & 1+\beta_{\xi32}^f & 0\end{pmatrix}.$$

To uniquely specify the Yukawa couplings g_ξ^f, we require that the parameters $\beta_{\xi mn}^f$ sum to zero:

$$\sum_{mn}\beta_{\xi mn}^f=0. \tag{6c}$$

When there is exact S_3 cyclic permutation symmetry the β's all vanish, and thus the case of approximate S_3 cyclic symmetry is parametrized by β's that are all small compared to unity. In a *CP*-conserving theory all of the coupling constants $g_{\phi,\eta}^f$ and all of the β's are real; when *CP* conservation is not imposed, these parameters can be complex.

We turn finally to the Higgs potential, which we separate into four terms as follows:

$$\mathcal{L}_{\text{Higgs potential}}=V_\phi+V_\eta+V_1(\phi,\eta)+V_2(\phi,\eta), \tag{7a}$$

with (for $\xi=\phi,\eta$)

$$V_\xi=\sum_{n=1}^{3}V_{\xi n},$$
$$V_{\xi n}=\lambda_{\xi n}(\xi_n^\dagger\xi_n-v_{\xi n}^2)^2 - \mu_{1\xi n}\xi_n^\dagger\xi_n\xi_{n+1}^\dagger\xi_{n+1}-\mu_{2\xi n}|\xi_n^\dagger\xi_{n+1}|^2 - \alpha_{\xi n}\text{Re}\exp(i\psi_{\xi n})\xi_n^\dagger\xi_{n+1}\xi_n^\dagger\xi_{n-1}, \tag{7b}$$

where the coefficients in Eq. (7b) are real (by Hermiticity) and where the parameter $\psi_{\xi n}$ is zero (modulo π) when CP conservation is imposed. For the potential terms that couple the ϕ and η Higgs fields, we have, in the *CP*-conserving case,

$$\begin{aligned}V_1(\phi,\eta)=\sum_{m,n=1}^{3}(&C_{1mn}\phi_m^\dagger\phi_m\eta_n^\dagger\eta_n+C_{2mn}\text{Re}\phi_m^\dagger\eta_m\eta_n^\dagger\phi_n\\ &+C_{3mn}\text{Re}\phi_m^\dagger\phi_{m+1}\eta_n^\dagger\eta_{n-1}\\ &+C_{4mn}\text{Re}\eta_m^\dagger\eta_{m+1}\phi_n^\dagger\phi_{n-1}\\ &+C_{5mn}\text{Re}\phi_m^\dagger\eta_{m+1}\eta_n^\dagger\phi_{n-1}\\ &+C_{6mn}\text{Re}\eta_m^\dagger\phi_{m+1}\phi_n^\dagger\eta_{n-1}),\end{aligned}$$

$$\begin{aligned}V_2(\phi,\eta)=\sum_n\ &\gamma_n\text{Re}\phi_n^\dagger\eta_n\\ &+\sum_{m,n=1}^{3}(C_{7mn}\text{Re}\phi_m^\dagger\phi_{m+1}\phi_n^\dagger\eta_{n-1}\\ &+C_{8mn}\text{Re}\phi_m^\dagger\phi_{m+1}\eta_n^\dagger\phi_{n-1}\\ &+C_{9mn}\text{Re}\eta_m^\dagger\eta_{m+1}\phi_n^\dagger\eta_{n-1}\\ &+C_{10mn}\text{Re}\eta_m^\dagger\eta_{m+1}\eta_n^\dagger\phi_{n-1}\\ &+C_{11mn}\text{Re}\phi_m^\dagger\eta_{m+1}\phi_n^\dagger\eta_{n-1}\\ &+C_{12mn}\text{Re}\eta_m^\dagger\phi_{m+1}\eta_n^\dagger\phi_{n-1}),\end{aligned} \tag{7c}$$

with all constants real (again by Hermiticity). The terms V_1 are those invariant under independent rephasings $\phi_n\to\exp(i\theta_\phi)\phi_n$ and $\eta_n\to\exp(i\theta_\eta)\eta_n$ of the two Higgs discrete chiral triplets, while the terms V_2 are only invariant under this phase transformation when restricted so that $\theta_\phi=\theta_\eta$. When *CP* is not conserved, an independent phase can be inserted inside each real part Re in the above expressions, in analogy with the construction of the final term of Eq. (7b). When there is S_3 cyclic permutation symmetry, the constants with a single discrete chiral subscript n are independent of that subscript, while the constants with a double subscript mn obey the cyclic condition $C_{lmn}=C_{lm+1n+1}$, $l=1,\ldots,12$.

This rather complicated Higgs potential completes the specification of our model, the tree approximation to which will be analyzed in detail in the sections that follow.

IV. RETROCIRCULANT AND CIRCULANT MATRICES

Before proceeding further, we pause to review the theory of circulant and retrocirculant matrices in the 3×3 case relevant for what follows. For a compact summary of general results see Marcus [7] and Hamburger and Grimshaw [7], and for a detailed exposition see Davis [8]. A matrix

$$\mathrm{Circ}_{\rightarrow}(a,b,c)\equiv\begin{pmatrix} a & b & c\\ c & a & b\\ b & c & a\end{pmatrix} \tag{8a}$$

is called a *circulant*, while a matrix

$$\mathrm{Circ}_{\leftarrow}(a,b,c)\equiv\begin{pmatrix} a & b & c\\ b & c & a\\ c & a & b\end{pmatrix} \tag{8b}$$

is called a *reverse circulant* or *retrocirculant*. [Clearly, a retrocirculant is always a symmetric matrix, and so $\mathrm{Circ}_{\leftarrow}(a,b,c)=\mathrm{Circ}_{\leftarrow}(a,b,c)^T$, and $\mathrm{Circ}_{\leftarrow}(a,b,c)^\dagger=\mathrm{Circ}_{\leftarrow}(a,b,c)^*$.] Two properties of these matrices are used in what follows. The first is that the Hermitian square of a retrocirculant is a circulant:

$$\begin{aligned}&\mathrm{Circ}_{\leftarrow}(a,b,c)\mathrm{Circ}_{\leftarrow}(a,b,c)^\dagger\\ &\quad=\mathrm{Circ}_{\rightarrow}(|a|^2+|b|^2+|c|^2,ab^*+bc^*+ca^*,\\ &\qquad ac^*+ba^*+cb^*),\\ &\mathrm{Circ}_{\leftarrow}(a,b,c)^\dagger\mathrm{Circ}_{\leftarrow}(a,b,c)\\ &\quad=\mathrm{Circ}_{\rightarrow}(|a|^2+|b|^2+|c|^2,\\ &\qquad a^*b+b^*c+c^*a,\\ &\qquad a^*c+b^*a+c^*b).\end{aligned} \tag{9}$$

The second is that any retrocirculant with arbitrary complex a,b,c is diagonalized by transformation from the left and right by unitary matrices U_L, $U_R=U_L^*$, which are independent of the values of a,b,c. Explicitly, setting

$$U_L=\frac{1}{\sqrt{3}}\begin{pmatrix}1 & \overline{\omega} & \omega\\ 1 & \omega & \overline{\omega}\\ 1 & 1 & 1\end{pmatrix},$$

$$U_R=\frac{1}{\sqrt{3}}\begin{pmatrix}1 & \omega & \overline{\omega}\\ 1 & \overline{\omega} & \omega\\ 1 & 1 & 1\end{pmatrix},$$

$$U_R^\dagger=\frac{1}{\sqrt{3}}\begin{pmatrix}1 & 1 & 1\\ \overline{\omega} & \omega & 1\\ \omega & \overline{\omega} & 1\end{pmatrix}, \tag{10a}$$

a simple calculation shows that

$$\begin{aligned}&U_L\mathrm{Circ}_{\leftarrow}(a,b,c)U_R^\dagger\\ &\quad=\begin{pmatrix}a+\overline{\omega}b+\omega c & 0 & 0\\ 0 & a+\omega b+\overline{\omega}c & 0\\ 0 & 0 & a+b+c\end{pmatrix}.\end{aligned} \tag{10b}$$

An elementary corollary of these statements is that any Hermitian circulant matrix $H_{\rightarrow}$ is diagonalized by the unitary transformation $U_L H_{\rightarrow} U_L^\dagger$ using the unitary matrix U_L of Eq. (10b).

The relevance of these results to what follows is that in the limit of S_3 cyclic permutation symmetry, we shall find that the fermion mass matrices in both the three- and six-doublet models are retrocirculants, and so are diagonalized by the universal bi-unitary transformation of Eq. (10b). By Eq. (9), the Hermitian squares of the fermion mass matrices in the approximation of cyclic permutation symmetry are therefore circulants, as suggested by Harrison and Scott [2]. We shall further find, in analyzing the Higgs sector in the case of cyclic permutation symmetry, that the Higgs boson mass matrices are also circulants, making it easy to diagonalize them explicitly.

V. STRUCTURE OF THE HIGGS SECTOR

We turn now to an analysis of the properties of the discrete chiral invariant Higgs potential of Eqs. (7a)–(7c). We shall assume *CP* invariance and exact S_3 cyclic permutation symmetry; when needed, we can take into account small deviations from these assumptions by adding perturbations to the locations of the Higgs minima. We begin our discussion with the three-Higgs-doublet model, in which only the discrete chiral triplet ϕ is present. Omitting the subscript ϕ on the coefficients, we have

$$\begin{aligned}&\mathcal{L}_{\text{Higgs potential}}\\ &\quad=\lambda\sum_{n=1}^{3}(\phi_n^\dagger\phi_n-v^2)^2-\mu_1\sum_{n=1}^{3}\phi_n^\dagger\phi_n\phi_{n+1}^\dagger\phi_{n+1}\\ &\qquad-\mu_2\sum_{n=1}^{3}|\phi_n^\dagger\phi_{n+1}|^2-\alpha\sum_{n=1}^{3}\mathrm{Re}\,\phi_n^\dagger\phi_{n+1}\phi_n^\dagger\phi_{n-1}.\end{aligned} \tag{11a}$$

Necessary conditions for this potential to be bounded below are evidently

$$\lambda>0,\quad \lambda-\mu_1-\mu_2-\alpha>0. \tag{11b}$$

Imposing the condition

$$\mu_2+\alpha>0 \tag{12a}$$

ensures that the Higgs potential is minimized when the three doublets all have the same form

$$\phi_n = \begin{pmatrix} 0 \\ \Omega_n \end{pmatrix}, \tag{12b}$$

for a suitable choice of SU(2) gauge, with the consequence that one electroweak gluon (the photon) remains massless. Imposing the additional condition

$$\alpha > 0 \tag{12c}$$

then forces the complex phases of the three expectations Ω_n to be equal (up to discrete chiral rephasings) at the minimum of the potential; by a choice of U(1) gauge the overall common phase can be rotated to zero, and so the potential of Eq. (11a) is minimized at

$$\Omega_1 = \Omega_2 = \Omega_3 = \Omega, \tag{13a}$$

with Ω given by

$$\Omega^2 = \frac{\lambda v^2}{\lambda - \mu_1 - \mu_2 - \alpha}. \tag{13b}$$

This minimum is not unique; because the potential of Eq. (11a) is invariant under the discrete chiral transformation of Eq. (3), equivalent minima are located at

$$\Omega_n = \omega_n \Omega, \quad n = 1,2,3, \tag{13c}$$

with $\omega_{1,2,3}$ any three distinct cube roots of unity, which can always be obtained by permutation from the set $\bar{\omega},\omega,1$. Despite the appearance of complex phases in Eq. (13c), there is no breakdown of *CP* invariance, because these phases can always be eliminated by the discrete chiral transformation that returns to the minimum of Eq. (13a).

We note that although the potential of Eq. (11a) is similar in form to that studied by Bigi and Sanda [9], they choose $\alpha < 0$, in which case there are nontrivial relative phases (that are not just discrete chiral rephasings) between the three expectations $\Omega_{1,2,3}$ at the potential minimum, and *CP* is spontaneously broken. This case is not useful for our model building because numerical analysis shows that it leads to a mass matrix with one heavy family, and two other lighter families of *equal* mass. We shall make use of the possibility [10] of *CP* violation in multi-Higgs-doublet systems only in the context of the six-doublet model, to be discussed shortly.

To complete our discussion of the three-doublet model, we must determine the Higgs masses. Expanding around the minimum of Eqs. (13a), (13b) to second order by substituting

$$\phi_n = \begin{pmatrix} \frac{1}{\sqrt{2}} \delta_n \\ \Omega + \frac{1}{\sqrt{2}} \epsilon_n \end{pmatrix} \tag{14a}$$

into Eq. (11a), we find

$$\mathcal{L}_{\text{Higgs potential}} = V_0 + V_{2\delta} + V_{2\epsilon},$$

$$V_{2\delta} = \sum_{m,n=1}^{3} \frac{1}{2} \delta_m^* B_{mn} \delta_n,$$

$$V_{2\epsilon} = \sum_{m,n=1}^{3} \frac{1}{2} [\epsilon_m^* A_{mn} \epsilon_n + \epsilon_m^* D_{mn} \epsilon_n^* + \epsilon_m D_{mn} \epsilon_n]. \tag{14b}$$

A simple calculation shows that the matrices A,B,D are all circulants of the form

$$A = \mathrm{Circ}_{\rightarrow}(a^A, b^A, b^A),$$

$$B = \mathrm{Circ}_{\rightarrow}(a^B, b^B, b^B),$$

$$D = \mathrm{Circ}_{\rightarrow}(a^D, b^D, b^D), \tag{15a}$$

with $a^{A,B,D}$ and $b^{A,B,D}$ given in terms of the Lagrangian parameters by

$$a^A = (2\lambda - \mu_1 - \mu_2) 2\Omega^2 - 2\lambda v^2,$$

$$b^A = -(\mu_1 + \mu_2 + 2\alpha)\Omega^2,$$

$$a^B = 2(\lambda - \mu_1)\Omega^2 - 2\lambda v^2,$$

$$b^B = -(\mu_2 + \alpha)\Omega^2,$$

$$a^D = \left(\lambda - \frac{1}{2}\alpha\right)\Omega^2,$$

$$b^D = -\frac{1}{4}(2\mu_1 + 2\mu_2 + \alpha)\Omega^2. \tag{15b}$$

Since these matrices are all diagonalized by transformations based on the cube roots of unity, it is useful to introduce new bases defined as follows:

$$\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = W \begin{pmatrix} \phi^{(1)} \\ \phi^{(2)} \\ \phi^{(3)} \end{pmatrix}, \quad \begin{pmatrix} \phi^{(1)} \\ \phi^{(2)} \\ \phi^{(3)} \end{pmatrix} = W^{-1} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix},$$

$$\begin{pmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \end{pmatrix} = W \begin{pmatrix} \delta^{(1)} \\ \delta^{(2)} \\ \delta^{(3)} \end{pmatrix}, \quad \begin{pmatrix} \delta^{(1)} \\ \delta^{(2)} \\ \delta^{(3)} \end{pmatrix} = W^{-1} \begin{pmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \end{pmatrix},$$

$$\begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \end{pmatrix} = W \begin{pmatrix} \epsilon^{(1)} \\ \epsilon^{(2)} \\ \epsilon^{(3)} \end{pmatrix}, \quad \begin{pmatrix} \epsilon^{(1)} \\ \epsilon^{(2)} \\ \epsilon^{(3)} \end{pmatrix} = W^{-1} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \end{pmatrix}, \tag{16a}$$

with

$$W=W^T=\frac{1}{\sqrt{3}}\begin{pmatrix}\omega & \overline{\omega} & 1\\ \overline{\omega} & \omega & 1\\ 1 & 1 & 1\end{pmatrix},$$

$$W^{-1}=W^\dagger=W^*=\frac{1}{\sqrt{3}}\begin{pmatrix}\overline{\omega} & \omega & 1\\ \omega & \overline{\omega} & 1\\ 1 & 1 & 1\end{pmatrix},$$

$$W^\dagger \mathrm{Circ}_{\rightarrow}(a,b,c)W = \begin{pmatrix} a+\omega b+\overline{\omega}c & 0 & 0\\ 0 & a+\overline{\omega}b+\omega c & 0\\ 0 & 0 & a+b+c\end{pmatrix},$$

$$W\mathrm{Circ}_{\rightarrow}(a,b,c)W = \begin{pmatrix} 0 & a+\overline{\omega}b+\omega c & 0\\ a+\omega b+\overline{\omega}c & 0 & 0\\ 0 & 0 & a+b+c\end{pmatrix}. \tag{16b}$$

In terms of the new bases, Eq. (14a) becomes

$$\phi^{(n)}=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta^{(n)}\\ \frac{1}{\sqrt{2}}\epsilon^{(n)}\end{pmatrix}, \quad n=1,2, \tag{16c}$$

and

$$\phi^{(3)}=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta^{(3)}\\ \sqrt{3}\Omega+\frac{1}{\sqrt{2}}\epsilon^{(3)}\end{pmatrix}. \tag{16d}$$

Substituting Eq. (16b) into both Eq. (14b) and the Higgs kinetic energy, and using Eq. (13b), we find, for the terms quadratic in δ_n,

$$\begin{aligned}&-\sum_{n=1,2,3}\frac{1}{2}|\partial_\mu\delta_n|^2+V_{2\delta}\\ &=-\sum_{n=1,2,3}\frac{1}{2}|\partial_\mu\delta^{(n)}|^2+(a^B+2b^B)\frac{1}{2}|\delta^{(3)}|^2\\ &\quad+(a^B-b^B)\frac{1}{2}(|\delta^{(1)}|^2+|\delta^{(2)}|^2)\\ &=-\sum_{n=1,2,3}\frac{1}{2}|\partial_\mu\delta^{(n)}|^2+\frac{3}{2}(\mu_2+\alpha)\Omega^2(|\delta^{(1)}|^2+|\delta^{(2)}|^2).\end{aligned} \tag{17a}$$

From Eq. (17a) we see that $\delta^{(3)}$ is a charged massless Goldstone boson (which is absorbed by the Higgs mechanism into the longitudinal parts of the charged intermediate bosons), while $\delta^{(1,2)}$ are two charged Higgs boson fields (each containing a positive and a negative charge state), with mass squared $3(\mu_2+\alpha)\Omega^2$. Similarly, we find, for the terms quadratic in ϵ_n,

$$\begin{aligned}&-\sum_{n=1,2,3}\frac{1}{2}|\partial_\mu\epsilon_n|^2+V_{2\epsilon}\\ &=-\sum_{n=1,2,3}\frac{1}{2}|\partial_\mu\epsilon^{(n)}|^2+(a^A+2b^A)\frac{1}{2}|\epsilon^{(3)}|^2\\ &\quad+(a^A-b^A)\frac{1}{2}(|\epsilon^{(1)}|^2+|\epsilon^{(2)}|^2)\\ &\quad+(a^D+2b^D)\frac{1}{2}[(\epsilon^{(3)})^2+(\epsilon^{(3)*})^2]\\ &\quad+(a^D-b^D)(\epsilon^{(1)}\epsilon^{(2)}+\epsilon^{(1)*}\epsilon^{(2)*}).\end{aligned} \tag{17b}$$

Defining new linear combinations $\epsilon^{(\pm)}$ by

$$\epsilon^{(\pm)}=\frac{1}{\sqrt{2}}(\epsilon^{(1)}\pm\epsilon^{(2)}), \tag{17c}$$

and splitting $\epsilon^{(3)},\epsilon^{(\pm)}$ into real and imaginary parts, $\epsilon^{(3,\pm)}=\epsilon_R^{(3,\pm)}+i\epsilon_I^{(3,\pm)}$, Eq. (17b) takes the form

$$\begin{aligned}&-\sum_{n=1,2,3}\frac{1}{2}|\partial_\mu\epsilon_n|^2+V_{2\epsilon}\\ &=-\frac{1}{2}[(\partial_\mu\epsilon_R^{(3)})^2+(\partial_\mu\epsilon_I^{(3)})^2+(\partial_\mu\epsilon_R^{(+)})^2+(\partial_\mu\epsilon_I^{(+)})^2\\ &\quad+(\partial_\mu\epsilon_R^{(-)})^2+(\partial_\mu\epsilon_I^{(-)})^2]+4\lambda v^2\frac{1}{2}(\epsilon_R^{(3)})^2\\ &\quad+\left(4\lambda+2\mu_1+2\mu_2+\frac{7}{2}\alpha\right)\Omega^2\frac{1}{2}[(\epsilon_R^{(+)})^2+(\epsilon_I^{(-)})^2]\\ &\quad+\frac{9}{2}\alpha\Omega^2\frac{1}{2}[(\epsilon_R^{(-)})^2+(\epsilon_I^{(+)})^2].\end{aligned} \tag{17d}$$

We see that $\epsilon_I^{(3)}$ is a neutral massless Goldstone boson (which is absorbed by the Higgs mechanism into the longitudinal part of the neutral intermediate boson), while $\epsilon_R^{(3)}$, both $\epsilon_R^{(+)}$ and $\epsilon_I^{(-)}$, and both $\epsilon_R^{(-)}$ and $\epsilon_I^{(+)}$ are neutral Higgs states, with respective squared masses $4\lambda v^2$, $(4\lambda+2\mu_1+2\mu_2+\frac{7}{2}\alpha)\Omega^2$, and $\frac{9}{2}\alpha\Omega^2$. Thus, the 12 states contained in the original triplet of Higgs doublets are accounted for as one neutral and two charged Goldstone modes, four charged Higgs bosons, and five neutral Higgs bosons. This information is summarized in Table I, which also gives the couplings of the Higgs bosons to fermions worked out in Sec. VI.

We turn next to the properties of the Higgs sector of the six-doublet model. Although we shall focus here on analytic

TABLE I. Higgs eigenmodes, masses, and fermion couplings for the three-Higgs-doublet model in the cyclic symmetry limit.

Mode designation	Charge	Mass squared	Fermion family couplings
$\delta^{(1)}$	± 1	$3(\mu_2+\alpha)\Omega^2$	First
$\delta^{(2)}$	± 1	$3(\mu_2+\alpha)\Omega^2$	Second
$\epsilon_R^{(3)}$	0	$4\lambda v^2$	Third
$\epsilon_R^{(+)},\epsilon_I^{(-)}$	0	$(4\lambda+2\mu_1+2\mu_2+\frac{7}{2}\alpha)\Omega^2$	First and second
$\epsilon_R^{(-)},\epsilon_I^{(+)}$	0	$\frac{9}{2}\alpha\Omega^2$	First and second

results, we have also made numerical studies of the minima of the six- (and three-) doublet potentials, using the formulas and method given in Appendix A. Let us begin by assuming that the potentials $V_1(\phi,\eta)$ and $V_2(\phi,\eta)$ of Eq. (7c), which couple the ϕ and η Higgs discrete chiral triplets, are very small. Then the minima of the Higgs potential are obtained by examining the degenerate minima of V_ϕ and V_η, as analyzed in the three-Higgs-doublet discussion above, and selecting those for which V_1+V_2 is smallest. By a simultaneous Z_6 rephasing of ϕ and η, we can always make the minimizing values of ϕ have the form of Eqs. (12b) and (13a), with Ω and the coefficients $\lambda,\ v,\ \alpha,\ \mu_1,\ \mu_2$ in Eq. (13b) now carrying the subscript ϕ to differentiate them from the similar formulas that hold for the Higgs field η. There are now two distinct possibilities, depending on the values of the coefficients in V_1 and V_2. Suppose, for example, that all of the coefficients γ_n, C_{lmn} in Eq. (7c) are negative; then V_1+V_2 is clearly minimized if the expectations of η_n are all relatively real to one another and to the expectations of ϕ_n, that is, if

$$\eta_n=\begin{pmatrix}0\\ \Lambda_n\end{pmatrix}, \tag{18a}$$

with

$$\Lambda_1=\Lambda_2=\Lambda_3=\Omega_\eta, \tag{18b}$$

with Ω_η given by Eq. (13b) with subscripts η on all quantities. Suppose, however, that the coefficients in V_1 and V_2 are all positive; then the sum V_1+V_2 will be made lower if we pick one of the degenerate minima of V_η of the form of Eq. (13c), for example,

$$\Lambda_1=\overline{\omega}\Omega_\eta,\quad \Lambda_2=\omega\Omega_\eta,\quad \Lambda_3=\Omega_\eta. \tag{18c}$$

More generally, the necessary condition for Eq. (18c) to be a lower minimum than Eq. (18b), in the limit of small coupling of η to ϕ, is that V_1+V_2 be smaller at Eq. (18c) than at Eq. (18b). Assuming exact cyclic permutation symmetry, which makes the following formulas independent of the value of the free index m, we find

$$\begin{aligned}V_1^{\text{Eq. (18b)}}&=3\Omega_\phi^2\Omega_\eta^2\sum_n\ (C_{1mn}+C_{2mn}+C_{3mn}+C_{4mn}\\&\quad+C_{5mn}+C_{6mn}),\end{aligned} \tag{19a}$$

$$\begin{aligned}V_2^{\text{Eq. (18b)}}&=3\gamma_m\Omega_\phi\Omega_\eta+3\sum_n\ [(C_{7mn}+C_{8mn})\Omega_\phi^3\Omega_\eta\\&\quad+(C_{9mn}+C_{10mn})\Omega_\eta^3\Omega_\phi\\&\quad+(C_{11mn}+C_{12mn})\Omega_\phi^2\Omega_\eta^2],\end{aligned}$$

and

$$\begin{aligned}V_1^{\text{Eq. (18c)}}&=3\Omega_\phi^2\Omega_\eta^2 C,\\ C&\equiv\left(\sum_n\left[C_{1mn}-\frac{1}{2}(C_{3mn}+C_{4mn})\right]\right)+C_{2mm}\\&\quad+C_{5m\,m+1}+C_{6m\,m+1}\\&\quad-\frac{1}{2}[C_{2m\,m+1}+C_{2m\,m-1}+C_{5mm}+C_{5m\,m-1}\\&\quad+C_{6mm}+C_{6m\,m-1}],\\ V_2^{\text{Eq. (18c)}}&=0.\end{aligned} \tag{19b}$$

Thus, the necessary condition for Eq. (18c) to be the minimum is that

$$V_1^{\text{Eq. (18c)}}<V_1^{\text{Eq. (18b)}}+V_2^{\text{Eq. (18b)}}. \tag{19c}$$

We shall henceforth assume that Eq. (19c) is satisfied; as already noted, this is automatic in the case when all of the coefficients in V_1 and V_2 are positive, but the general condition is much less restrictive, requiring only that the coefficients lie on one side of a hyperplane in the space of $V_{1,2}$ coefficients. When Eq. (19c) is satisfied, *CP* invariance is spontaneously broken through the η Higgs expectations, and we shall see in the next section that simultaneously, the η expectations have the correct form to generate nonzero second family masses.

Let us next consider what happens when V_1 and V_2 are not infinitesimally small. Still maintaining cyclic permutation invariance, let us first consider the case in which V_1 is large, but V_2 remains nearly zero. Then, from the formulas of Appendix A, we find that the derivatives of the potential vanish when one assumes Eq. (13a) for the ϕ expectations (with Ω of course replaced by Ω_ϕ) and Eq. (18c) for the η expectations, for suitable minimizing values of Ω_ϕ and Ω_η. In other words, we find the correct minimum by first substituting Eqs. (13a) and (18c) into the Higgs potential, and then minimizing the resulting simplified expression with respect to Ω_ϕ and Ω_η. Substituting Eqs. (13a) and (18c) into Eq. (7a) gives

$$\begin{aligned}\tfrac{1}{3}\mathcal{L}_{\text{Higgs potential}}&=A_\phi\Omega_\phi^4-2B_\phi\Omega_\phi^2+A_\eta\Omega_\eta^4-2B_\eta\Omega_\eta^2\\&\quad+C\Omega_\phi^2\Omega_\eta^2+\text{const},\end{aligned} \tag{20a}$$

with C given in Eq. (19b), and with the remaining coefficients given by

$$A_\xi=\lambda_\xi-\mu_{1\xi}-\mu_{2\xi}-\alpha_\xi, \quad B_\xi=\lambda_\xi v_\xi^2, \quad \xi=\phi,\eta. \tag{20b}$$

Minimizing Eq. (20a) with respect to $\Omega_\phi^2,\Omega_\eta^2$ gives a pair of simultaneous linear equations, with the solution

$$\Omega_\phi^2=\frac{A_\eta B_\phi-\frac{1}{2}CB_\eta}{A_\phi A_\eta-\frac{1}{4}C^2}, \quad \Omega_\eta^2=\frac{A_\phi B_\eta-\frac{1}{2}CB_\phi}{A_\phi A_\eta-\frac{1}{4}C^2}. \tag{20c}$$

In order for both ϕ and η to develop nonzero vacuum expectation values we must have $\Omega_\phi^2>0$, $\Omega_\eta^2>0$, which in the case when the denominator in Eq. (20c) is positive requires that C be restricted by

$$-2A_\phi^{1/2}A_\eta^{1/2}<C<2\,\mathrm{Min}\left(\frac{A_\phi}{B_\phi}B_\eta,\frac{A_\eta}{B_\eta}B_\phi,A_\phi^{1/2}A_\eta^{1/2}\right). \tag{20d}$$

Because V_1 is invariant under independent overall phase rotations of ϕ and η, in the limit when V_2 is strictly zero the minimum of Eqs. (13a) and (18c) is part of a one-parameter U(1) family of equivalent minima, of the form

$$(\Omega_1,\Omega_2,\Omega_3)=(1,1,1)\Omega_\phi,$$

$$(\Lambda_1,\Lambda_2,\Lambda_3)=(\bar{\omega},\omega,1)\Omega_\eta \exp(i\theta), \tag{21}$$

with the angle θ arbitrary. When V_2 is nonzero but very small, the U(1) degeneracy with respect to θ is broken, and the minimum has the form of Eq. (21) with a definite value of θ determined by the Higgs Lagrangian parameters. A perturbative analysis in powers of V_2 shows that to first order in V_2 the degeneracy in θ is unbroken [because the final line of Eq. (19b) remains valid for general θ], but that at second order in V_2 a nontrivial condition on θ is obtained and the degeneracy is broken. Numerical minimization of the Higgs potential, using the method of Appendix A, shows that general values of θ can be attained at the minimum for generic Lagrangian parameters. As V_2 increases, there are relative phase and small magnitude corrections to the minima of Eq. (21); when the assumption of cyclic permutation symmetry is relaxed, these magnitude corrections become more pronounced.

To conclude our discussion of the six-Higgs-doublet model, let us discuss the Higgs boson mass spectrum, assuming both exact cyclic permutation symmetry and the weak coupling limit in which both V_1 and V_2 are very small. We parametrize the expansion of ϕ_n and η_n around the minimum as

$$\phi_n=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta_n^\phi\\ \Omega_\phi+\frac{1}{\sqrt{2}}\epsilon_n^\phi\end{pmatrix}, \tag{22a}$$

$$\eta_n=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta_n^\eta\\ \Omega_\eta+\frac{1}{\sqrt{2}}\epsilon_n^\eta\end{pmatrix}\exp(i\theta)(\bar{\omega},\omega,1)_n, \tag{22b}$$

where we have used the notation $(x,y,z)_n$ to indicate x for $n=1$, y for $n=2$, and z for $n=3$. Because the overall phase θ and the discrete chiral phases $(\bar{\omega},\omega,1)_n$ drop out of V_η, for the non-Goldstone modes we get simply two copies of the nonzero mass modes found in Eqs. (17a)–(17d) in the three-Higgs-doublet case, apart from adding subscripts or superscripts ϕ,η to distinguish the ϕ and η sectors, as summarized in Table II. In computing the Yukawa couplings of the η_n Higgs modes, the phases in Eq. (22b) play a role. Making transformations analogous to Eqs. (16a) in the three-Higgs-doublet case, with ξ in the following formulas either ϕ or η, we have

$$\begin{pmatrix}\xi_1\\ \xi_2\\ \xi_3\end{pmatrix}=W\begin{pmatrix}\xi^{(1)}\\ \xi^{(2)}\\ \xi^{(3)}\end{pmatrix}, \quad \begin{pmatrix}\xi^{(1)}\\ \xi^{(2)}\\ \xi^{(3)}\end{pmatrix}=W^{-1}\begin{pmatrix}\xi_1\\ \xi_2\\ \xi_3\end{pmatrix},$$

$$\begin{pmatrix}\delta_1^\xi\\ \delta_2^\xi\\ \delta_3^\xi\end{pmatrix}=W\begin{pmatrix}\delta_\xi^{(1)}\\ \delta_\xi^{(2)}\\ \delta_\xi^{(3)}\end{pmatrix}, \quad \begin{pmatrix}\delta_\xi^{(1)}\\ \delta_\xi^{(2)}\\ \delta_\xi^{(3)}\end{pmatrix}=W^{-1}\begin{pmatrix}\delta_1^\xi\\ \delta_2^\xi\\ \delta_3^\xi\end{pmatrix},$$

$$\begin{pmatrix}\epsilon_1^\xi\\ \epsilon_2^\xi\\ \epsilon_3^\xi\end{pmatrix}=W\begin{pmatrix}\epsilon_\xi^{(1)}\\ \epsilon_\xi^{(2)}\\ \epsilon_\xi^{(3)}\end{pmatrix}, \quad \begin{pmatrix}\epsilon_\xi^{(1)}\\ \epsilon_\xi^{(2)}\\ \epsilon_\xi^{(3)}\end{pmatrix}=W^{-1}\begin{pmatrix}\epsilon_1^\xi\\ \epsilon_2^\xi\\ \epsilon_3^\xi\end{pmatrix}. \tag{23}$$

In terms of the new bases, Eq. (22a) becomes

$$\phi^{(n)}=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta_\phi^{(n)}\\ \frac{1}{\sqrt{2}}\epsilon_\phi^{(n)}\end{pmatrix}, \quad n=1,2, \tag{24a}$$

and

$$\phi^{(3)}=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta_\phi^{(3)}\\ \sqrt{3}\Omega_\phi+\frac{1}{\sqrt{2}}\epsilon_\phi^{(3)}\end{pmatrix}, \tag{24b}$$

TABLE II. Higgs eigenmodes, masses, and fermion couplings for the six-Higgs-doublet model in the cyclic symmetry limit, assuming weak coupling of ϕ to η.

Mode designation	Charge	Mass squared	Fermion family couplings
$\delta_\phi^{(1)}$	± 1	$3(\mu_{2\phi}+\alpha_\phi)\Omega_\phi^2$	First
$\delta_\phi^{(2)}$	± 1	$3(\mu_{2\phi}+\alpha_\phi)\Omega_\phi^2$	Second
$\epsilon_{\phi R}^{(3)}$	0	$4\lambda_\phi v_\phi^2$	Third
$\epsilon_{\phi R}^{(+)},\epsilon_{\phi I}^{(-)}$	0	$(4\lambda_\phi+2\mu_{1\phi}+2\mu_{2\phi}+\frac{7}{2}\alpha_\phi)\Omega_\phi^2$	First and second
$\epsilon_{\phi R}^{(-)},\epsilon_{\phi I}^{(+)}$	0	$\frac{9}{2}\alpha_\phi\Omega_\phi^2$	First and second
$\delta_\eta^{(1)}$	± 1	$3(\mu_{2\eta}+\alpha_\eta)\Omega_\eta^2$	Third
$\delta_\eta^{(2)}$	± 1	$3(\mu_{2\eta}+\alpha_\eta)\Omega_\eta^2$	First
$\epsilon_{\eta R}^{(3)}$	0	$4\lambda_\eta v_\eta^2$	Second
$\epsilon_{\eta R}^{(+)},\epsilon_{\eta I}^{(-)}$	0	$(4\lambda_\eta+2\mu_{1\eta}+2\mu_{2\eta}+\frac{7}{2}\alpha_\eta)\Omega_\eta^2$	First and third
$\epsilon_{\eta R}^{(-)},\epsilon_{\eta I}^{(+)}$	0	$\frac{9}{2}\alpha_\eta\Omega_\eta^2$	First and third
$\delta_{PG}^{(3)}$	± 1	$\sim\|V_2\|/\Omega^2$	Second and third
$\epsilon_{PG}^{(3)}$	0	$\sim\|V_2\|/\Omega^2$	Second and third

while taking into account the extra phases, Eq. (22b) becomes

$$\eta^{(3)}=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta_\eta^{(1)}\\ \frac{1}{\sqrt{2}}\epsilon_\eta^{(1)}\end{pmatrix}\exp(i\theta), \tag{24c}$$

$$\eta^{(1)}=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta_\eta^{(2)}\\ \frac{1}{\sqrt{2}}\epsilon_\eta^{(2)}\end{pmatrix}\exp(i\theta), \tag{24d}$$

and

$$\eta^{(2)}=\begin{pmatrix}\frac{1}{\sqrt{2}}\delta_\eta^{(3)}\\ \sqrt{3}\Omega_\eta+\frac{1}{\sqrt{2}}\epsilon_\eta^{(3)}\end{pmatrix}\exp(i\theta). \tag{24e}$$

The fact that Ω_η appears in $\eta^{(2)}$ rather than in $\eta^{(3)}$ is directly related, as we shall see in the next section, to the role of the η Higgs bosons in giving rise to second family masses.

For the Goldstone modes, the situation is more complicated, because the ϕ and η sectors interact even in the weak coupling limit. If V_2 were exactly zero, as noted above we would have an extra U(1) symmetry, and we would get two copies of the Goldstone modes as well. But for nonzero V_2 this U(1) degeneracy is broken, and we are left with just one set of Goldstone modes, corresponding to the remaining invariance of the Higgs potential under simultaneous overall rephasing of ϕ,η, while the three Goldstone modes related to the relative phase θ of ϕ and η become massive pseudo Goldstone modes, with squared masses that are proportional to the magnitude of V_2. The decomposition of $\delta_{\phi,\eta}^{(3)}$ and $\epsilon_{I\phi,\eta}^{(3)}$ into Goldstone and pseudo Goldstone modes is made unique by the facts that (i) these represent orthogonal degrees of freedom, which are simply rotations from the original modes $\delta_{\phi,\eta}^{(3)}$ and $\epsilon_{I\phi,\eta}^{(3)}$, and (ii) the Goldstone modes correspond precisely to a uniform infinitesimal phase rotation of ϕ,η, which specifies the infinitesimal modes to which the pseudo Goldstone modes must be orthogonalized. Since the expectations of ϕ,η may have unequal magnitudes Ω_ϕ,Ω_η, we see from Eqs. (24a)–(24d) that an overall infinitesimal phase rotation makes a contribution to $\delta_\eta^{(3)}$ that is Ω_η/Ω_ϕ times as large as the corresponding contribution to $\delta_\phi^{(3)}$, and similarly makes a contribution to $\epsilon_{I\eta}^{(3)}$ that is Ω_η/Ω_ϕ times as large as the corresponding contribution to $\epsilon_{I\phi}^{(3)}$. We thus find, denoting the Goldstone and pseudo Goldstone modes, respectively, by the subscripts G and PG, and as before using the subscript I to denote the imaginary part,

$$\delta_G^{(3)}=\frac{\Omega_\phi\delta_\phi^{(3)}+\Omega_\eta\delta_\eta^{(3)}}{(\Omega_\phi^2+\Omega_\eta^2)^{1/2}},\quad \delta_{PG}^{(3)}=\frac{\Omega_\eta\delta_\phi^{(3)}-\Omega_\phi\delta_\eta^{(3)}}{(\Omega_\phi^2+\Omega_\eta^2)^{1/2}}, \tag{25a}$$

$$\epsilon_G^{(3)}=\frac{\Omega_\phi\epsilon_{I\phi}^{(3)}+\Omega_\eta\epsilon_{I\eta}^{(3)}}{(\Omega_\phi^2+\Omega_\eta^2)^{1/2}},\quad \epsilon_{PG}^{(3)}=\frac{\Omega_\eta\epsilon_{I\phi}^{(3)}-\Omega_\phi\epsilon_{I\eta}^{(3)}}{(\Omega_\phi^2+\Omega_\eta^2)^{1/2}}.$$

The corresponding quadratic terms in the Lagrangian are

$$-\frac{1}{2}[|\partial_\mu\delta_{\rm G}^{(3)}|^2+|\partial_\mu\delta_{\rm PG}^{(3)}|^2+(\partial_\mu\epsilon_{\rm G}^{(3)})^2+(\partial_\mu\epsilon_{\rm PG}^{(3)})^2]$$
$$+\frac{1}{2}[M^2_{\text{charged PG}}|\delta_{\rm PG}^{(3)}|^2+M^2_{\text{neutral PG}}(\epsilon_{\rm PG}^{(3)})^2]. \tag{25b}$$

The perturbative contribution to the pseudo Goldstone boson masses, relative to the Higgs boson masses calculated above, will have the general magnitude (suppressing all subscripts)

$$\frac{M_{\rm PG}}{M_{\rm Higgs}}\sim\left(\frac{|V_2|}{\lambda\Omega^4}\right)^{1/2}. \tag{25c}$$

We have not attempted to calculate explicit perturbative formulas for the pseudo Goldstone boson masses, both because these will be rather complicated given the complexity of V_2 and because, as argued by Weinberg [11], there are likely to be significant nonperturbative corrections of order gM_W, with g the electroweak gauge coupling and M_W the electroweak boson mass.

VI. HIGGS COUPLINGS AND MASS AND CKM MATRICES WHEN CYCLIC PERMUTATION SYMMETRY IS EXACT

We proceed now to study the Yukawa couplings of the Higgs fields, and the mass matrices generated by their vacuum expectation values, when cyclic permutation symmetry is exact. Thus, in this section we shall assume that the Higgs potentials have the cyclically symmetric form analyzed in detail in Sec. V, and we shall take the asymmetry parameters $\beta^f_{\xi lm}$ of Eqs. (6b), (6c) to vanish. As a consequence, the 3×3 matrices $P^f_{\xi n}$ of Eq. (6b) are all retrocirculants, and are independent of the labels ξ, f:

$$P^f_{\xi1}=\mathrm{Circ}_\leftarrow(0,1,0),$$
$$P^f_{\xi2}=\mathrm{Circ}_\leftarrow(0,0,1),$$
$$P^f_{\xi3}=\mathrm{Circ}_\leftarrow(1,0,0). \tag{26}$$

Substituting Eq. (23) for $\xi_{1,2,3}$, with $\xi=\phi,\eta$, into the first line of Eq. (6a), we get, for $f=d,e$,

$$\Phi^f=g^f_\phi(P^{f(1)}_\phi\phi^{(1)}+P^{f(2)}_\phi\phi^{(2)}+P^{f(3)}_\phi\phi^{(3)})$$
$$+g^f_\eta(P^{f(1)}_\eta\eta^{(1)}+P^{f(2)}_\eta\eta^{(2)}+P^{f(3)}_\eta\eta^{(3)}). \tag{27a}$$

Here we have defined

$$\begin{pmatrix}P^{f(1)}_\xi\\ P^{f(2)}_\xi\\ P^{f(3)}_\xi\end{pmatrix}=W\begin{pmatrix}P^f_{\xi1}\\ P^f_{\xi2}\\ P^f_{\xi3}\end{pmatrix}=W^{-1}\begin{pmatrix}P^f_{\xi2}\\ P^f_{\xi1}\\ P^f_{\xi3}\end{pmatrix}, \tag{27b}$$

with W and W^{-1} as given in Eq. (16b). Defining CP conjugates of $\xi^{(1,2,3)}$ by

$$\tilde{\xi}^{(1,2,3)}=i\tau_2\xi^{(1,2,3)*}, \tag{28a}$$

the CP conjugate of the first group of equations in Eq. (23) is

$$\begin{pmatrix}\tilde\xi_1\\ \tilde\xi_2\\ \tilde\xi_3\end{pmatrix}=W^{-1}\begin{pmatrix}\tilde\xi^{(1)}\\ \tilde\xi^{(2)}\\ \tilde\xi^{(3)}\end{pmatrix},\begin{pmatrix}\tilde\xi^{(1)}\\ \tilde\xi^{(2)}\\ \tilde\xi^{(3)}\end{pmatrix}=W\begin{pmatrix}\tilde\xi_1\\ \tilde\xi_2\\ \tilde\xi_3\end{pmatrix}. \tag{28b}$$

Using this for $\phi_{1,2,3}$, $\eta_{1,2,3}$ in the second line of Eq. (6a), we get, for $f=u,\nu$,

$$\Phi^f=g^f_\phi(P^{f(1)}_\phi\tilde\phi^{(1)}+P^{f(2)}_\phi\tilde\phi^{(2)}+P^{f(3)}_\phi\tilde\phi^{(3)})$$
$$+g^f_\eta(P^{f(1)}_\eta\tilde\eta^{(1)}+P^{f(2)}_\eta\tilde\eta^{(2)}+P^{f(3)}_\eta\tilde\eta^{(3)}). \tag{28c}$$

Substituting the retrocirculant forms of Eq. (26) into Eq. (27b), we can write the matrices $P^{f(1,2,3)}_\xi$ as retrocirculants:

$$P^{f(1)}_\xi=\frac{1}{\sqrt3}\mathrm{Circ}_\leftarrow(1,\omega,\overline{\omega}),$$
$$P^{f(2)}_\xi=\frac{1}{\sqrt3}\mathrm{Circ}_\leftarrow(1,\overline{\omega},\omega),$$
$$P^{f(3)}_\xi=\frac{1}{\sqrt3}\mathrm{Circ}_\leftarrow(1,1,1). \tag{29a}$$

Let us now use Eq. (10b), which asserts that $P^{f(1,2,3)}_\xi$ are all diagonalized by the same bi-unitary transformation constructed using $U_L, U_R^\dagger$ of Eq. (10a):

$$U_LP^{f(1)}_\xi U_R^\dagger=\sqrt3\,\mathrm{diag}(1,0,0)\equiv\sqrt3M^{(1)},$$
$$U_LP^{f(2)}_\xi U_R^\dagger=\sqrt3\,\mathrm{diag}(0,1,0)\equiv\sqrt3M^{(2)},$$
$$U_LP^{f(3)}_\xi U_R^\dagger=\sqrt3\,\mathrm{diag}(0,0,1)\equiv\sqrt3M^{(3)}. \tag{29b}$$

Clearly, the natural thing to do now is to rotate to new fermion bases using the same matrices U_L, U_R, by introducing primed bases defined by

$$Q_L=U_L^\dagger Q_L',\quad \psi_L=U_L^\dagger\psi_L',$$
$$f_R=U_R^\dagger f_R',\quad f=d,u,e,\nu. \tag{30a}$$

Since the fermion kinetic energy of Eq. (4c) does not couple left to right chiral components, it has the same form in terms of the primed bases as in terms of the original ones. Substituting Eqs. (27a), (28c), and (29b) into the Yukawa Lagrangian of Eq. (5b), we get finally

$$\mathcal{L}_{\rm Yukawa}=\overline{Q}_L'\Psi^d d_R'+\overline{Q}_L'\Psi^u u_R'+\overline{\psi}_L'\Psi^e e_R'+\overline{\psi}_L'\Psi^\nu\nu_R'$$
$$+\text{adjoint}, \tag{30b}$$

with the 3×3 matrices Ψ^f defined by

$$\Psi^f=\sum_{l=1}^{3} \sqrt{3}(g_\phi^f \phi^{(l)}+g_\eta^f \eta^{(l)})M^{(l)}, \quad f=d,e,$$

$$\Psi^f=\sum_{l=1}^{3} \sqrt{3}(g_\phi^f \tilde{\phi}^{(l)}+g_\eta^f \tilde{\eta}^{(l)})M^{(l)}, \quad f=u,\nu. \tag{30c}$$

On substituting Eqs. (24a)–(24d) into Eq. (30c), we can read off both the mass matrices and the Yukawa couplings of the physical Higgs states. The mass matrices are obtained by keeping only the vacuum expectations of $\phi^{(l)}, \eta^{(l)}$, that is, by setting

$$\phi^{(1,2)}\to 0, \quad \tilde{\phi}^{(1,2)}\to 0,$$

$$\phi^{(3)}\to \begin{pmatrix} 0 \\ \sqrt{3}\Omega_\phi \end{pmatrix}, \quad \tilde{\phi}^{(3)}\to \begin{pmatrix} \sqrt{3}\Omega_\phi \\ 0 \end{pmatrix}, \tag{31a}$$

and

$$\eta^{(1,3)}\to 0, \quad \tilde{\eta}^{(1,3)}\to 0,$$

$$\eta^{(2)}\to \begin{pmatrix} 0 \\ \sqrt{3}\Omega_\eta \exp(i\theta) \end{pmatrix}, \quad \tilde{\eta}^{(2)}\to \begin{pmatrix} \sqrt{3}\Omega_\eta \exp(-i\theta) \\ 0 \end{pmatrix}, \tag{31b}$$

giving

$$\begin{aligned}\mathcal{L}_{\rm mass}=&\overline{d}_L'[3g_\eta^d\Omega_\eta \exp(i\theta)M^{(2)}+3g_\phi^d\Omega_\phi M^{(3)}]d_R'\\ &+\overline{u}_L'[3g_\eta^u\Omega_\eta \exp(-i\theta)M^{(2)}+3g_\phi^u\Omega_\phi M^{(3)}]u_R'\\ &+\overline{e}_L'[3g_\eta^e\Omega_\eta \exp(i\theta)M^{(2)}+3g_\phi^e\Omega_\phi M^{(3)}]e_R'\\ &+\overline{\nu}_L'[3g_\eta^\nu\Omega_\eta \exp(-i\theta)M^{(2)}+3g_\phi^\nu\Omega_\phi M^{(3)}]\nu_R'\\ &+\text{adjoint}.\end{aligned} \tag{32a}$$

Identifying $M^{(1,2,3)}$, respectively, as the projectors on the first, second, and third family states in the primed basis, we read off from Eq. (32a) the masses

$$\begin{aligned}&M_t=3g_\phi^u\Omega_\phi, \quad M_c=3g_\eta^u\Omega_\eta, \quad M_u=0,\\ &M_b=3g_\phi^d\Omega_\phi, \quad M_s=3g_\eta^d\Omega_\eta, \quad M_d=0,\\ &M_\tau=3g_\phi^e\Omega_\phi, \quad M_\mu=3g_\eta^e\Omega_\eta, \quad M_e=0,\\ &M_{\nu_\tau}=3g_\phi^\nu\Omega_\phi, \quad M_{\nu_\mu}=3g_\eta^\nu\Omega_\eta, \quad M_{\nu_e}=0.\end{aligned} \tag{32b}$$

We see that in the three-Higgs-doublet model, only the third family gets masses, with the first two families remaining massless. The same is true in the *CP*-conserving phase of the six-Higgs-doublet model, in which the η expectations are given by Eq. (18b) rather than Eq. (18c); in this phase, the projectors $M^{(2)}$ in Eq. (32a) are replaced by projectors $M^{(3)}$, and the η expectations simply make additional contributions to the third family masses. On the other hand, in the phase of the six-Higgs-doublet model that spontaneously violates *CP* as in Eqs. (18c) and (21), the factors $\overline{\omega},\omega,1$ in Eq. (18c) give rise to the projector $M^{(2)}$ for the second family states, which then receive masses. The hierarchy between the masses of the second and third family charged leptons is attributed, in the six-Higgs-doublet model, to a systematic tendency of the η Higgs bosons to have smaller Yukawa couplings to the charged fermions than those of the ϕ Higgs bosons.

To get a feeling for the magnitudes involved, we note that the Higgs boson expectations generate mass terms for the gauge bosons given by

$$\mathcal{L}_{\rm gauge\ mass}=\left[-\frac{g^2}{4}W_{+\mu}W_{-\mu}-\frac{1}{8}(gW_{3\mu}-g'B_\mu)^2\right]v^2, \tag{33a}$$

with

$$v^2=2\sum_{n=1}^{3}(|\langle\phi_n\rangle|^2+|\langle\eta_n\rangle|^2)=6(\Omega_\phi^2+\Omega_\eta^2). \tag{33b}$$

Empirically, $v\simeq 247$ GeV; assuming, as we shall in the fits below, that Ω_ϕ and Ω_η are approximately equal, we then find $\Omega_\phi\simeq\Omega_\eta\simeq 71$ GeV. The Yukawa couplings needed to reproduce the observed charged fermion masses are then given in the six-Higgs-doublet model by

$$\begin{aligned}&g_\phi^u\simeq 0.81, \quad g_\eta^u\simeq 0.0061,\\ &g_\phi^d\simeq 0.020, \quad g_\eta^d\simeq 0.00094,\\ &g_\phi^e\simeq 0.0083, \quad g_\eta^e\simeq 0.0005.\end{aligned} \tag{34a}$$

In the three-Higgs-doublet model, Ω_ϕ is a factor of $\sqrt{2}$ larger than in the six-Higgs-doublet model, and the ϕ Yukawa couplings are correspondingly a factor of $\sqrt{2}$ smaller than in Eq. (34a):

$$g_\phi^u\simeq 0.57, \quad g_\phi^d\simeq 0.014, \quad g_\phi^e\simeq 0.0059. \tag{34b}$$

As we have seen, because the mass matrices in the cyclically symmetric limit are retrocirculants, we were able to diagonalize them with universal, flavor-independent matrices U_L, U_R. This has the important consequence that when cyclic symmetry is assumed as a leading approximation, the corresponding approximation to the CKM mixing matrix is unity, a welcome feature since the observed CKM matrix is close to unity. A related welcome feature of the cyclic approximation is that there are no flavor-changing neutral currents, which again accords with the fact that these are observed to be highly suppressed. To obtain realistic nonunit values for the CKM matrix, we will have to go beyond the cyclic approximation by including nonzero asymmetries

$\beta^f_{\xi lm}$ as in Eq. (6b), but we shall then also have to estimate the magnitude of the flavor-changing neutral current effects produced by these asymmetries. This will be the agenda of the next three sections.

Before proceeding with this analysis, we note that the leading cyclic approximation to the Yukawa couplings of the physical Higgs bosons can be read off from Eqs. (30b), (30c) together with Eqs. (24a)–(24d) and (25a). We see that

$$\begin{aligned} &\delta_\phi^{(1)}, \quad \epsilon_\phi^{(1)}, \quad \delta_\eta^{(2)}, \quad \epsilon_\eta^{(2)} \quad \text{couple only to the first family,}\\ &\delta_\phi^{(2)}, \quad \epsilon_\phi^{(2)}, \quad \delta_\eta^{(3)}, \quad \epsilon_\eta^{(3)} \quad \text{couple only to the second family,}\\ &\delta_\phi^{(3)}, \quad \epsilon_\phi^{(3)}, \quad \delta_\eta^{(1)}, \quad \epsilon_\eta^{(1)} \quad \text{couple only to the third family,} \end{aligned} \tag{35a}$$

which by Eq. (17c) imply that

$$\begin{aligned} &\epsilon^{(\pm)}_{\phi R,I} \quad \text{couple only to the first and second families,}\\ &\epsilon^{(\pm)}_{\eta R,I} \quad \text{couple only to the first and third families,} \end{aligned} \tag{35b}$$

and by Eq. (25a) imply that

$$\delta^{(3)}_{PG}, \quad \epsilon^{(3)}_{PG} \quad \text{couple only to the second and third families.} \tag{35c}$$

The presence of 21 Higgs bosons in the six-Higgs-doublet model (eight charged Higgs bosons $\delta^{(1,2)}_{\phi,\eta}$ and ten neutral Higgs bosons $\epsilon^{(3)}_{R\phi,\eta}$, $\epsilon^{(\pm)}_{R\phi,\eta}$, and $\epsilon^{(\pm)}_{I\phi,\eta}$, plus two charged pseudo Goldstone Higgs bosons $\delta^{(3)}_{PG}$, and one neutral pseudo Goldstone Higgs boson $\epsilon^{(3)}_{PG}$), together with the pattern of predominant fermionic couplings given in Eqs. (35a)–(35c) and summarized in Table II, is a distinguishing feature of the model that should be testable in experiments at the next generation of accelerators.

VII. FIRST ORDER BREAKING OF CYCLIC PERMUTATION SYMMETRY

We now set up a perturbative scheme to study the effects of the breaking of cyclic permutation symmetry. In the three-Higgs-doublet model, we will also allow CP noninvariance of the Lagrangian, by allowing the phases ψ in Eq. (7b) to be nonzero and by allowing the Yukawa couplings to be complex. In the six-Higgs-doublet model, we will impose *CP* invariance on the Lagrangian, but will work in the phase that spontaneously breaks *CP*. Two types of first order small corrections will be introduced. The first are corrections to the Higgs vacuum expectations, arising from a lack of cyclic symmetry in the Higgs potential. In the three-Higgs-doublet model, this results in replacing Eq. (13a) by

$$\Omega_n = \Omega(1+\delta_n), \quad n=1,2,3, \tag{36a}$$

where the δ_n are small corrections that can be complex, and where we impose the condition

$$\sum_n \delta_n = 0 \tag{36b}$$

to avoid duplicating information contained in the overall factor Ω and the overall phase that has been eliminated by a gauge transformation. In the six-Higgs-doublet model, we have analogous corrections to the first line in Eq. (21):

$$\Omega_n = \Omega_\phi(1+\delta_n), \quad n=1,2,3, \ \sum_n \delta_n = 0, \tag{37}$$

where the δ_n can again be complex when the potentials V_1, V_2 that couple ϕ to η are not neglected. In principle, there are also asymmetry corrections to the second line of Eq. (21), which gives the η expectations. But these are always suppressed by a factor g^f_η/g^f_ϕ, which according to Eq. (34a) is at most of order 0.06, and so will be neglected in what follows; that is, we treat g_η/g_ϕ here as if it were also a first order small quantity. The second type of first order small corrections are the asymmetry parameters $\beta^f_{\phi mn}$ of Eqs. (6b), (6c), which are complex in the three-Higgs-doublet model when explicit *CP* violation is permitted, but are real in the six-Higgs-doublet model when *CP* invariance is imposed on the Lagrangian. Again, in principle there are analogous asymmetry parameters $\beta^f_{\eta mn}$ for the η Yukawa couplings, but the effect of these is again suppressed by a factor g^f_η/g^f_ϕ and so they will be neglected. This itemization of corrections defines the model that we shall study in first order perturbation theory.

Since the zeroth order problem, which was analyzed in Sec. VI, is brought to diagonal form by the bi-unitary transformations of Eqs. (29b) and (30a) based on the matrices U_L, U_R of Eq. (10a), we shall make this transformation at the outset. In the primed fermion basis, the zeroth order mass matrix is still given by Eq. (32a), but now there will be first order corrections from the δ's and β's introduced above. Since we are regarding g^f_η/g^f_ϕ as effectively a first order correction, it is convenient to group it with the other first order terms. Starting again from Eqs. (23), (27a), (27b), and (28c), we then find, for the extension of Eq. (32a) to include all first order corrections,

$$\mathcal{L}_{\rm mass} = \sum_{f=d,u,e,\nu} \overline{f'_L} g^f_\phi \Omega_\phi (3M^{(3)} + \sigma^f) f'_R, \tag{38a}$$

with σ^f a 3×3 matrix with matrix elements given by

$$\sigma_{11}^f=\frac{1}{3}\mu_{11}^f+\delta_3^f+\overline{\omega}\delta_2^f+\omega\delta_1^f,$$

$$\sigma_{22}^f=\frac{1}{3}\mu_{22}^f+3R^f+\delta_3^f+\omega\delta_2^f+\overline{\omega}\delta_1^f,$$

$$\sigma_{33}^f=0,$$

$$\sigma_{lm}^f=\frac{1}{3}\mu_{lm}^f, \quad l\neq m. \tag{38b}$$

The further quantities appearing in Eq. (38b) are defined as follows. The quantities δ_n^f are given, in terms of the δ_n introduced in Eqs. (36) and (37), by

$$\delta_1^f=\delta_2, \quad \delta_2^f=\delta_1, \quad \delta_3^f=\delta_3, \quad f=d,e,$$

$$\delta_1^f=\delta_1^*, \quad \delta_2^f=\delta_2^*, \quad \delta_3^f=\delta_3^*, \quad f=u,\nu. \tag{39a}$$

The quantities R^f are defined by

$$R^f=\frac{g_\eta^f\Omega_\eta\exp(\pm i\theta)}{g_\phi^f\Omega_\phi}, \tag{39b}$$

with the $+$ sign holding for $f=d,e$ and the $-$ sign holding for $f=u,\nu$. Finally, the μ_{lm}^f's, when multiplied by the factor of 1/3 in Eq. (38b), are the asymmetries $\beta_{\phi lm}^f$ reexpressed in the primed fermion basis; suppressing the subscript ϕ on the β's, they are given by

$$\mu_{11}^f=\beta_{11}^f+\beta_{23}^f+\beta_{32}^f+\overline{\omega}(\beta_{12}^f+\beta_{21}^f+\beta_{33}^f)$$
$$+\omega(\beta_{13}^f+\beta_{22}^f+\beta_{31}^f),$$

$$\mu_{22}^f=\beta_{11}^f+\beta_{23}^f+\beta_{32}^f+\omega(\beta_{12}^f+\beta_{21}^f+\beta_{33}^f)$$
$$+\overline{\omega}(\beta_{13}^f+\beta_{22}^f+\beta_{31}^f),$$

$$\mu_{12}^f=\beta_{11}^f+\beta_{22}^f+\beta_{33}^f+\omega(\beta_{12}^f+\beta_{23}^f+\beta_{31}^f)$$
$$+\overline{\omega}(\beta_{21}^f+\beta_{32}^f+\beta_{13}^f),$$

$$\mu_{21}^f=\beta_{11}^f+\beta_{22}^f+\beta_{33}^f+\overline{\omega}(\beta_{12}^f+\beta_{23}^f+\beta_{31}^f)$$
$$+\omega(\beta_{21}^f+\beta_{32}^f+\beta_{13}^f),$$

$$\mu_{13}^f=\beta_{11}^f+\beta_{12}^f+\beta_{13}^f+\overline{\omega}(\beta_{21}^f+\beta_{22}^f+\beta_{23}^f)$$
$$+\omega(\beta_{31}^f+\beta_{32}^f+\beta_{33}^f),$$

$$\mu_{23}^f=\beta_{11}^f+\beta_{12}^f+\beta_{13}^f+\omega(\beta_{21}^f+\beta_{22}^f+\beta_{23}^f)$$
$$+\overline{\omega}(\beta_{31}^f+\beta_{32}^f+\beta_{33}^f),$$

$$\mu_{31}^f=\beta_{11}^f+\beta_{21}^f+\beta_{31}^f+\overline{\omega}(\beta_{12}^f+\beta_{22}^f+\beta_{32}^f)$$
$$+\omega(\beta_{13}^f+\beta_{23}^f+\beta_{33}^f),$$

$$\mu_{32}^f=\beta_{11}^f+\beta_{21}^f+\beta_{31}^f+\omega(\beta_{12}^f+\beta_{22}^f+\beta_{32}^f)$$
$$+\overline{\omega}(\beta_{13}^f+\beta_{23}^f+\beta_{33}^f). \tag{39c}$$

We remark that since *CP* invariance requires the β's to be real, the condition for *CP* invariance, when expressed directly in terms of the μ's, is $\mu_{11}^{f*}=\mu_{22}^f$, $\mu_{12}^{f*}=\mu_{21}^f$, $\mu_{13}^{f*}=\mu_{23}^f$, and $\mu_{31}^{f*}=\mu_{32}^f$.

Defining

$$M_f'\equiv 3M^{(3)}+\sigma^f, \tag{40a}$$

we must now find the bi-unitary transformation matrices U_L^f, U_R^f for which $U_L^f M_f' U_R^{f\dagger}$ is diagonal, with the eigenvalues ordered in absolute value, for each flavor f. The fermion basis states that are mass eigenstates are then related to the primed basis by

$$f_L'=U_L^{f\dagger}f_L^{\mathrm{mass}},$$

$$f_R'=U_R^{f\dagger}f_R^{\mathrm{mass}}, \quad f=d,u,e,\nu, \tag{40b}$$

and the CKM matrix U_{CKM} is given as usual by

$$U_{\mathrm{CKM}}=U_L^{u\dagger}U_L^d. \tag{40c}$$

We shall now develop a perturbative procedure for calculating $U_{L,R}^f$. The first observation to be made is that we are dealing with a degenerate perturbation problem, since the zeroth order mass matrix $3M^{(3)}=3\,\mathrm{diag}(0,0,1)$ has eigenvalues 0 for the first two primed basis states. As a consequence, the 2×2 submatrix of $U_{L,R}^f$ spanned by these states is zeroth order in the perturbation σ^f, with only the off-diagonal elements coupling to the third basis state of first order. Thus, we find a natural reason in our model why the CKM mixings of the first and second family states should be larger than the mixings of the first and second families with the third family.

We shall deal with the zeroth order 2×2 submatrix by calculating it exactly. Let $V_{L,R}^f$ be the 2×2 matrices that bring the 2×2 submatrix of σ^f to diagonal form:

$$V_L^f\begin{pmatrix}\sigma_{11}^f & \sigma_{12}^f\\ \sigma_{21}^f & \sigma_{22}^f\end{pmatrix}V_R^{f\dagger}=\begin{pmatrix}\kappa_1^f & 0\\ 0 & \kappa_2^f\end{pmatrix}, \tag{41a}$$

with the magnitudes of the eigenvalues ordered as $|\kappa_1^f|\leqslant|\kappa_2^f|$. The explicit construction of $V_{L,R}^f$ is given in Appendix B. It is then straightforward to show that to first order in small quantities, $U_{L,R}^f$ are given by

$$U_L^f=\begin{pmatrix} V_L^f & -\frac{1}{3}V_L^f\begin{pmatrix}\sigma_{13}^f\\ \sigma_{23}^f\end{pmatrix}\\ \frac{1}{3}\begin{pmatrix}\sigma_{13}^f\\ \sigma_{23}^f\end{pmatrix}^\dagger & 1\end{pmatrix}, \tag{41b}$$

$$U_R^{f\dagger}=\begin{pmatrix} V_R^{f\dagger} & \frac{1}{3}\begin{pmatrix}\sigma_{31}^{f*}\\ \sigma_{32}^{f*}\end{pmatrix}\\ -\frac{1}{3}\begin{pmatrix}\sigma_{31}^{f*}\\ \sigma_{32}^{f*}\end{pmatrix}^{\dagger}V_R^{f\dagger} & 1\end{pmatrix}, \tag{41c}$$

and

$$U_L^f M_f' U_R^{f\dagger}=\begin{pmatrix}\kappa_1^f & 0 & 0\\ 0 & \kappa_2^f & 0\\ 0 & 0 & 3\end{pmatrix}. \tag{41d}$$

Defining

$$V_{\rm CKM}\equiv V_L^{u\dagger}V_L^d, \tag{42a}$$

the corresponding first order accurate expression for the CKM matrix is given by

$$U_{\rm CKM}=\begin{pmatrix} V_{\rm CKM} & -\frac{1}{3}V_{\rm CKM}\begin{pmatrix}\sigma_{13}^d\\ \sigma_{23}^d\end{pmatrix}+\frac{1}{3}\begin{pmatrix}\sigma_{13}^u\\ \sigma_{23}^u\end{pmatrix}\\ \frac{1}{3}\begin{pmatrix}\sigma_{13}^d\\ \sigma_{23}^d\end{pmatrix}^{\dagger}-\frac{1}{3}\begin{pmatrix}\sigma_{13}^u\\ \sigma_{23}^u\end{pmatrix}^{\dagger}V_{\rm CKM} & 1\end{pmatrix}. \tag{42b}$$

Although Eq. (42b) is useful for analytic study of the CKM matrix, in our numerical work we shall simply compute directly from the definition of Eq. (40c). We shall also, in the numerical work, use slightly more accurate forms for $U_{L,R}^f$ in which only the square of the ratio of second to third family masses $(|\kappa_2^f|/3)^2$ is assumed to be small; the relevant formulas are given in Appendix C.

VIII. HIGGS BOSON EXCHANGE CONTRIBUTIONS TO THE K_L-K_S MASS DIFFERENCE

As pointed out in Sec. VI, when cyclic symmetry is exact, Higgs boson exchange in our models does not produce strangeness-changing neutral current effects. However, once we include cyclic asymmetries, such effects become possible and we must be sure that their magnitude does not exceed known experimental limits. Since, in the context of extensions of the Higgs sector, the most stringent bound on strangeness-changing neutral current processes comes [13] from the second order weak K_L-K_S mass difference, we shall consider only this process, and shall calculate the contribution to its matrix element arising from Higgs boson exchange within the perturbative framework set up in Sec. VII.

We saw there that, because the zeroth order mass matrix is degenerate in the subspace spanned by the first two families, the mixing matrices within this subspace are *zeroth order* rather than first order in the perturbation, and therefore strangeness-changing neutral current effects can already appear at zeroth order in perturbation theory. What we shall do in this section is to calculate this zeroth order contribution to the K_L-K_S mass difference, neglecting all terms of first and higher order in the asymmetric perturbation. Our starting point is thus the Yukawa Lagrangian of Eqs. (30b), (30c) in the primed basis, of which the term relevant to mixing of the d and s quarks is

$$\overline{Q}_L'\sum_{l=1}^{3}\sqrt{3}(g_\phi^d\phi^{(l)}+g_\eta^d\eta^{(l)})M^{(l)}d_R'+\text{adjoint}. \tag{43a}$$

Substituting Eq. (40b) relating the primed to the mass eigenstate bases and using the approximation of Eqs. (41b), (41c) for $U_{L,R}^d$; also substituting Eqs. (24a), (24b) for the $\phi^{(l)}$ and keeping only the neutral Higgs pieces, and finally also neglecting terms of first and higher order in the asymmetric perturbation, we get the effective Lagrangian

$$\mathcal{L}_{\rm scnc}\equiv\overline{d}_L^{\rm mass}\frac{\sqrt{3}}{\sqrt{2}}g_\phi^d\sum_{l=1}^{2}\epsilon_\phi^{(l)}V_L^dM_{2\times2}^{(l)}V_R^{d\dagger}d_R^{\rm mass}+\text{adjoint}. \tag{43b}$$

In Eq. (43b), the subscript 2×2 on the projectors indicates their restriction to the subspace spanned by the first two families, and the column vector d will be understood to have been truncated from three to two components, corresponding to the first two families. Finally, reexpressing $\epsilon_\phi^{(1,2)}$ in terms of the modes $\epsilon_\phi^{(\pm)}$ defined in Eq. (17c), splitting these into real and imaginary parts, and explicitly including the adjoint term [our γ matrix conventions are $\gamma_5=\gamma_5^\dagger$, $\gamma^0=\gamma^{0\dagger}$, $(\gamma^0)^2=1$], we get

$$\mathcal{L}_{\rm scnc}=\bar{d}^{\rm mass}\frac{\sqrt{3}}{4}g_\phi^d\{[(\epsilon_{\phi R}^{(+)}+\epsilon_{\phi R}^{(-)})+i(\epsilon_{\phi I}^{(+)}+\epsilon_{\phi I}^{(-)})]V_L^d M_{2\times 2}^{(1)}V_R^{d\dagger}+[(\epsilon_{\phi R}^{(+)}-\epsilon_{\phi R}^{(-)})+i(\epsilon_{\phi I}^{(+)}-\epsilon_{\phi I}^{(-)})]V_L^d M_{2\times 2}^{(2)}V_R^{d\dagger}\}$$
$$\times(1+\gamma_5)d^{\rm mass}+\bar{d}^{\rm mass}\frac{\sqrt{3}}{4}g_\phi^{d*}\{[(\epsilon_{\phi R}^{(+)}+\epsilon_{\phi R}^{(-)})-i(\epsilon_{\phi I}^{(+)}+\epsilon_{\phi I}^{(-)})]V_R^d M_{2\times 2}^{(1)}V_L^{d\dagger}$$
$$+[(\epsilon_{\phi R}^{(+)}-\epsilon_{\phi R}^{(-)})-i(\epsilon_{\phi I}^{(+)}-\epsilon_{\phi I}^{(-)})]V_R^d M_{2\times 2}^{(2)}V_L^{d\dagger}\}(1-\gamma_5)d^{\rm mass}. \tag{43c}$$

To facilitate the remaining calculation, it is convenient to rewrite Eq. (43c) in the form

$$\mathcal{L}_{\rm scnc}=\bar{d}^{\rm mass}\epsilon_{\phi R}^{(+)}(A_R^{(+)}+B_R^{(+)}\gamma_5)d^{\rm mass}+\bar{d}^{\rm mass}\epsilon_{\phi R}^{(-)}(A_R^{(-)}+B_R^{(-)}\gamma_5)d^{\rm mass}$$
$$+\bar{d}^{\rm mass}\epsilon_{\phi I}^{(+)}(A_I^{(+)}+B_I^{(+)}\gamma_5)d^{\rm mass}+\bar{d}^{\rm mass}\epsilon_{\phi I}^{(-)}(A_I^{(-)}+B_I^{(-)}\gamma_5)d^{\rm mass}. \tag{44a}$$

Using the fact that

$$M_{2\times 2}^{(1)}+M_{2\times 2}^{(2)}=\begin{pmatrix}1&0\\0&1\end{pmatrix}\equiv 1,\quad M_{2\times 2}^{(1)}-M_{2\times 2}^{(2)}=\begin{pmatrix}1&0\\0&-1\end{pmatrix}\equiv\rho_3, \tag{44b}$$

we find that the 2×2 matrices $A_{R,I}^{(\pm)}$, $B_{R,I}^{(\pm)}$ appearing in Eq. (44a) are given by

$$A_R^{(+)}=\frac{\sqrt{3}}{4}g_\phi^d V_L^d V_R^{d\dagger}+\frac{\sqrt{3}}{4}g_\phi^{d*}V_R^d V_L^{d\dagger},\quad B_R^{(+)}=\frac{\sqrt{3}}{4}g_\phi^d V_L^d V_R^{d\dagger}-\frac{\sqrt{3}}{4}g_\phi^{d*}V_R^d V_L^{d\dagger},$$
$$A_R^{(-)}=\frac{\sqrt{3}}{4}g_\phi^d V_L^d\rho_3 V_R^{d\dagger}+\frac{\sqrt{3}}{4}g_\phi^{d*}V_R^d\rho_3 V_L^{d\dagger},\quad B_R^{(-)}=\frac{\sqrt{3}}{4}g_\phi^d V_L^d\rho_3 V_R^{d\dagger}-\frac{\sqrt{3}}{4}g_\phi^{d*}V_R^d\rho_3 V_L^{d\dagger}, \tag{44c}$$
$$A_I^{(+)}=\frac{\sqrt{3}}{4}g_\phi^d iV_L^d V_R^{d\dagger}-\frac{\sqrt{3}}{4}g_\phi^{d*}iV_R^d V_L^{d\dagger},\quad B_I^{(+)}=\frac{\sqrt{3}}{4}g_\phi^d iV_L^d V_R^{d\dagger}+\frac{\sqrt{3}}{4}g_\phi^{d*}iV_R^d V_L^{d\dagger},$$
$$A_I^{(-)}=\frac{\sqrt{3}}{4}g_\phi^d iV_L^d\rho_3 V_R^{d\dagger}-\frac{\sqrt{3}}{4}g_\phi^{d*}iV_R^d\rho_3 V_L^{d\dagger},\quad B_I^{(-)}=\frac{\sqrt{3}}{4}g_\phi^d iV_L^d\rho_3 V_R^{d\dagger}+\frac{\sqrt{3}}{4}g_\phi^{d*}iV_R^d\rho_3 V_L^{d\dagger}. \tag{44d}$$

Letting d and s denote, respectively, the down and strange quark eigenstates, the two component column vector $d^{\rm mass}$ has the structure

$$d^{\rm mass}=\begin{pmatrix}d\\s\end{pmatrix}, \tag{45a}$$

and so for any 2×2 matrix N, we have

$$\bar{d}^{\rm mass}Nd^{\rm mass}=\bar{d}N_{11}d+\bar{d}N_{12}s+\bar{s}N_{21}d+\bar{s}N_{22}s. \tag{45b}$$

Hence the strangeness-changing terms of Eq. (44a) involve only the 12 and 21 matrix elements of the matrices in Eq. (44c), and can be compactly written as

$$\mathcal{L}_{\rm scnc}^{\Delta S=1}=\sum_{p=\pm}\sum_{F=R,I}[\bar{d}\epsilon_{\phi F}^{(p)}(A_{F12}^{(p)}+B_{F12}^{(p)}\gamma_5)s$$
$$+\bar{s}\epsilon_{\phi F}^{(p)}(A_{F21}^{(p)}+B_{F21}^{(p)}\gamma_5)d]. \tag{45c}$$

So for the amplitude T for the $\Delta S=2$ process $s+s\to d+d$ we find, summing over the exchanges of Higgs eigenmodes $\epsilon_{\phi F}^{(p)}$ with squared masses $M_F^{2(p)}$, the formula (valid up to an overall phase)

$$T=\sum_{p=\pm}\sum_{F=R,I}\bar{d}(A_{F12}^{(p)}+B_{F12}^{(p)}\gamma_5)s\frac{1}{M_F^{2(p)}}$$
$$\times\bar{d}(A_{F12}^{(p)}+B_{F12}^{(p)}\gamma_5)s, \tag{46a}$$

while from Sec. V and Table II we find, for the squared masses,

$$M_R^{2(+)}=M_I^{2(-)}=(4\lambda_\phi+2\mu_{1\phi}+2\mu_{2\phi}+\tfrac{7}{2}\alpha_\phi)\Omega_\phi^2,$$

$$M_R^{2(-)}=M_I^{2(+)}=\tfrac{9}{2}\alpha_\phi\Omega_\phi^2,\quad\Omega_\phi^2=\frac{\lambda_\phi v_\phi^2}{\lambda_\phi-\mu_{1\phi}-\mu_{2\phi}-\alpha_\phi}. \tag{46b}$$

The Higgs boson exchange matrix element $\langle K|T|\overline{K}\rangle_{\rm Higgs}$ for the $\overline{K}\rightarrow K$ transition, in the vacuum saturation approximation, then is given by

$$|\langle K|T|\overline{K}\rangle_{\rm Higgs}|\simeq N|\langle K|\overline{d}\gamma_5 s|0\rangle|^2|D_{\rm Higgs}|, \tag{47a}$$

with $D_{\rm Higgs}$ given by

$$D_{\rm Higgs}=\sum_{p=\pm}\sum_{F=R,I}\frac{(B_{F12}^{(p)})^2}{M_F^{2(s)}}, \tag{47b}$$

and with $N=8/3$ a Wick contraction and color factor.

We wish now to compare the amplitude of Eq. (47a) with the intermediate boson loop diagram contribution to the K_L-K_S mass difference calculated by Gaillard and Lee [14], which in the vacuum saturation approximation is in satisfactory agreement with experiment. The Gaillard-Lee result is

$$|\langle K|T|\overline{K}\rangle_{\rm GL}|\simeq N|\langle K|\overline{d}\gamma_\mu\gamma_5 s|0\rangle|^2|D_{\rm GL}|, \tag{48a}$$

with $|D_{\rm GL}|$ given by

$$|D_{\rm GL}|=\frac{G_F^2}{4\pi^2}M_c^2 s_{12}^2, \tag{48b}$$

in terms of the Fermi constant G_F, the charm quark mass M_c, and the sine of the Cabibbo angle $s_{12}=\sin\theta_C$. To compare Eq. (47a) to Eq. (48a), we need the ratio of the pseudoscalar current to the axial vector current kaon to vacuum matrix elements, which can be estimated by standard current algebra methods (see, e.g., Shuryak [15]) to be

$$\frac{|\langle K|\overline{d}\gamma_5 s|0\rangle|^2}{|\langle K|\overline{d}\gamma_\mu\gamma_5 s|0\rangle|^2}\simeq\frac{\langle 0|\overline{u}u|0\rangle^2}{M_K^2 f_K^4}\simeq\left(\frac{M_K}{M_s}\right)^2\simeq 11, \tag{49}$$

with M_K and f_K the kaon mass and decay constant and with M_s the strange quark mass. Combining everything, we find that the condition for the Higgs boson exchange contribution to the K_L-K_S mass difference not to exceed the Gaillard-Lee estimate is

$$|D_{\rm Higgs}|\leqslant\frac{G_F^2M_c^2M_s^2s_{12}^2}{4\pi^2M_K^2}\simeq\frac{2.6\times10^{-14}}{\rm GeV^2}, \tag{50}$$

which will be used as the strangeness-changing neutral current constraint in the fits of the next section.

IX. NUMERICAL FITS OF THE THREE- AND SIX-HIGGS-DOUBLET MODELS TO THE EXPERIMENTAL DATA

In order to fit the models to the experimental data, we follow the standard procedure of minimizing a ‘‘cost function’’ C, constructed as follows:

$$C=C_{\rm mass}+C_{\rm CKM}+C_{\rm scnc}+C_{\rm parameter}, \tag{51a}$$

with the pieces referring, respectively, to the constraints placed by fitting the masses, fitting the CKM mixing angles, obeying the strangeness-changing neutral current bound of Eq. (50), and keeping the asymmetry parameters as small as possible. Before giving further details, we describe the general search method employed. We perform all fits using the minimization routine POWELL of Press *et al.* [12]. As given in [12], this routine works well for the six-Higgs-doublet model where the degeneracy between the first and second families is already broken, before inclusion of the asymmetry parameters, by the η Higgs couplings. However, in the three-Higgs-doublet model, it is not *a priori* specified which states become the first and which become the second families, and so eigenvalue crossings can occur in the course of the iteration which result in discontinuous behavior of the cost function. This causes a problem with the bracketing routine MNBRAK of [12], which occasionally gets stuck in an indefinite loop. The fix is simply putting an iteration counter into MNBRAK, to force an exit with a default bracketing (specifically, in terms of the quantities defined in MNBRAK, $c=a$, $fc=fa$) if convergence to a bracketing is not attained in $N_{\rm max}$ passes through the loop. We found the same results in the three-Higgs-doublet model with $N_{\rm max}=5$ as with $N_{\rm max}=30$, indicating that a bracketing is attained very rapidly, or not at all. As an additional check, we verified that the original and the modified versions of MNBRAK give identical results for the six-Higgs-doublet model, where level crossings and associated discontinuous behavior do not occur.

Let us now turn to the construction of the various cost function terms in Eq. (51a), working throughout in units where 1 GeV = unity. For the mass cost function, we use a standard chi-squared function constructed from expected values of the masses and their estimated errors, including the electroweak mass parameter v of Eq. (33b). To prevent the chi squared for certain very accurately known masses (such as the electron mass) from dominating the fits, we truncate these masses to a few significant figures and use enlarged error estimates. In the six-Higgs-doublet model we also add a term that favors fits with $\Omega_\phi\simeq\Omega_\eta$, since this degeneracy plays a role in the extension to neutrino mixings discussed in the next section; in practice, we find that this term has very little effect on the fits, since nearly equal values of Ω_ϕ and Ω_η are favored even in its absence. (This term is omitted in the three-Higgs-doublet model, where it is not relevant.) Adding these contributions, we have, for the mass cost function $C_{\rm mass}$,

$$\begin{aligned}C_{\rm mass}=&\left(\frac{M_u-0.005}{0.003}\right)^2+\left(\frac{M_c-1.3}{0.18}\right)^2+\left(\frac{M_t-173.0}{6.0}\right)^2\\&+\left(\frac{M_d-0.01}{0.005}\right)^2+\left(\frac{M_s-0.2}{0.06}\right)^2+\left(\frac{M_b-4.3}{0.2}\right)^2\\&+\left(\frac{M_e-0.00051}{0.0001}\right)^2+\left(\frac{M_\mu-0.1057}{0.001}\right)^2\\&+\left(\frac{M_\tau-1.777}{0.001}\right)^2+\left(\frac{[6(\Omega_\phi^2+\Omega_\eta^2)]^{1/2}-247.0}{3.0}\right)^2\\&+(\Omega_\phi-\Omega_\eta)^2.\end{aligned} \tag{51b}$$

For the strangeness-changing neutral current cost function, we use a chi-squared function with expectation zero and standard deviation equal to the bound of Eq. (50):

$$C_{\rm scnc} = \left(\frac{|D_{\rm Higgs}|}{2.6 \times 10^{-14}} \right)^2 . \tag{51c}$$

To set up the CKM cost function, we make the standard rephasings to put the CKM matrix in the form

$$U_{\rm CKM} = \begin{pmatrix} 1 & s_{12} & s_{13} e^{-i\delta_{13}} \\ -s_{12} & 1 & s_{23} \\ -s_{13} e^{i\delta_{13}} & -s_{23} & 1 \end{pmatrix}, \tag{52a}$$

to first order accuracy in small quantities, and then construct a chi-squared function from the expected values and estimated errors for s_{12}, s_{13}, and s_{23}. Although the *CP*-violating angle δ_{13} has not been reliably determined experimentally, it appears likely that it is appreciable; so we also include a chi-squared term requiring $|\sin \delta_{13}|$ to be equal to 0.6 ± 0.3, giving

$$C_{\rm CKM} = \left(\frac{s_{12} - 0.221}{0.002} \right)^2 + \left(\frac{s_{13} - 0.0035}{0.0009} \right)^2 + \left(\frac{s_{23} - 0.041}{0.003} \right)^2 + \left(\frac{|\sin \delta_{13}| - 0.6}{0.3} \right)^2 . \tag{52b}$$

Altogether, then, there are 11 quantities to be fitted in $C_{\rm mass}$, 1 to be fitted in $C_{\rm scnc}$, and 4 to be fitted in $C_{\rm CKM}$, for a total of 16.

Let us now count the numbers of parameters in the two models, and establish the cost functions for the parameters. Despite its increased complexity in terms of particle content, the six-Higgs-doublet model has the smaller number of parameters, since it violates *CP* only spontaneously and so all Yukawa couplings appearing in the Lagrangian are real. Altogether, there are 37 parameters that enter into the iterative fit for the six-Higgs-doublet model. These are the ϕ and η expectations Ω_ϕ and Ω_η, the real parts of the Yukawa couplings $g^f_{\phi,\eta}$, $f = u,d,e$, the complex asymmetry parameters $\delta_{1,2}$ introduced in Eq. (37), the angle θ of Eqs. (21) and (39b), and the real asymmetry parameters $\beta^f_{\phi mn}$, $f = u,d,e$, $m+n<6$ introduced in Eqs. (6b), (6c). The parameters λ_ϕ, $\mu_{1\phi} + \mu_{2\phi}$, and α_ϕ, which enter the calculation only through their appearance in the Higgs boson masses in the strangeness-changing neutral current constraint [see Eqs. (46), (47)], were fixed at the respective values 1, 0.3, and 0.3, and were not iterated. To construct the cost function for the iterated parameters, we note that no additional constraint is needed for the expectations $\Omega_{\phi,\eta}$ or the Yukawa couplings $g^f_{\phi,\eta}$ because these are already adequately controlled by $C_{\rm mass}$ of Eq. (51b). For the remaining parameters we use the cost function

$$C_{\rm parameter} = \sum_{n=1,2} \left| \frac{\delta_n}{\sigma_{\rm parameter}} \right|^\epsilon + \sum_{\substack{m,n \; m+n<6 \\ f=u,d,e}} \left| \frac{\beta^f_{\phi mn}}{\sigma_{\rm parameter}} \right|^\epsilon + \left| \frac{\theta}{6.28} \right|^\epsilon . \tag{53a}$$

In Eq. (53a) the exponent ϵ and the width $\sigma_{\rm parameter}$ are parameters of the fitting procedure, which effectively set up a model for how the small asymmetries are distributed. We were able to get satisfactory fits for both $\epsilon = 1$ and $\epsilon = 2$, but convergence was much slower for the latter, suggesting that $\epsilon = 1$ is a model in closer correspondence to the experimental data, and we shall only present the $\epsilon = 1$ results in the discussion below. To initialize the six-Higgs-doublet minimization search, we started from $\Omega_\eta = \Omega_\phi = 70.7$, the values of Eq. (34a) for the Yukawa couplings $g^f_{\phi,\eta}$, zero for the asymmetry parameters $\delta_n, \beta^f_{\phi mn}$, and zero for θ.

Because the three-Higgs-doublet model, to give a *CP*-violating CKM matrix, must violate *CP* explicitly, its Yukawa couplings and Yukawa asymmetries can have imaginary parts, and so there are 57 parameters that enter into the iterative fit. These are the ϕ expectation Ω_ϕ, the real parts of the Yukawa couplings g^f_ϕ, $f = u,d,e$, and the imaginary part of g^d_ϕ (since $g^{u,e}_\phi$, which are not involved in the strangeness-changing neutral current constraint, enter only through their absolute values, they can be rephased to be real), the complex asymmetry parameters $\delta_{1,2}$ introduced in Eq. (36a), and the complex asymmetry parameters $\beta^f_{\phi mn}$, $f = u,d,e$, $m+n<6$, introduced in Eqs. (6b), (6c). Again, the parameters λ_ϕ, $\mu_{1\phi} + \mu_{2\phi}$, and α_ϕ, which enter the calculation only through the strangeness-changing neutral current constraint, were fixed at the respective values 1, 0.3, and 0.3. To construct the cost function for the iterated parameters, we note that again no additional constraint is needed for the expectation Ω_ϕ or the real parts of the Yukawa couplings g^f_ϕ, because these are adequately controlled by $C_{\rm mass}$ of Eq. (51b). For the remaining parameters we use the cost function

$$C_{\rm parameter} = \sum_{\substack{n=1,2 \\ F=R,I}} \left| \frac{\delta_{nF}}{\sigma_{\rm parameter}} \right|^\epsilon + \sum_{\substack{m,n \; m+n<6 \\ f=u,d,e \\ F=R,I}} \left| \frac{\beta^f_{\phi mnF}}{\sigma_{\rm parameter}} \right|^\epsilon + \left| \frac{g^d_{\phi I}}{0.028} \right|^\epsilon . \tag{53b}$$

The width 0.028 governing $g^d_{\phi I}$ is chosen here as twice the natural magnitude of g^d_ϕ according to the estimate of Eq. (34b), so as to bound $g^d_{\phi I}$ but not overly restrict it, much as the width for θ in the six-Higgs-doublet model is chosen in Eq. (53a) as twice the maximum magnitude π of $|\theta|$. Again, the exponent ϵ and the width $\sigma_{\rm parameter}$ are parameters that model how the small asymmetries are distributed. For comparison with the six-Higgs-doublet model fits, we shall again only present $\epsilon = 1$ results in the discussion that follows. To initialize the three-Higgs-doublet minimization search, we started from $\Omega_\phi = 100$, the values of Eq. (34b) for the real

TABLE III. Six-Higgs-doublet model fit to experimental data

Quantity	Target value	Fitted value
$v=[6(\Omega_\phi^2+\Omega_\eta^2)]^{1/2}$	247.0	247.0
$\Omega_\phi-\Omega_\eta$	0.0	0.001
M_u	0.005	0.005
M_c	1.30	1.28
M_t	173.0	173.0
M_d	0.010	0.011
M_s	0.200	0.219
M_b	4.30	4.29
M_e	0.00051	0.00051
M_μ	0.1057	0.1057
M_τ	1.777	1.777
$\frac{\lvert D_{\rm Higgs}\rvert}{2.6\times 10^{-14}}$	0.0	0.016
s_{12}	0.221	0.221
s_{13}	0.0035	0.0041
s_{23}	0.041	0.035
$\lvert\sin\delta_{13}\rvert$	0.60	0.44

parts of the Yukawa couplings g_ϕ^f, zero for the imaginary part of g_ϕ^d, and zero for the complex asymmetry parameters $\delta_n, \beta_{\phi mn}^f$.

We begin by presenting results for the six-Higgs-doublet model. In any fitting procedure involving more parameters than quantities to be fit, one has to worry about overfitting, and we deal with this in the following way. As we shall see shortly, the most sensitive aspect of the fitting procedure for the six-Higgs-doublet model is getting the CKM parameters correct, and so we take the cost function subcomponent $C_{\rm CKM}$ as a measure of overfitting. Making a series of fits using the cost function of Eq. (53a) with $\epsilon=1$, as a function of the width $\sigma_{\rm parameter}$, we find that the value of $C_{\rm CKM}$ is a monotonic decreasing function of the width. For very small values of the width (i.e., asymmetries restricted to have very small values) we find a value of $C_{\rm CKM}$ much larger than 4, the number of fitted CKM matrix degrees of freedom; for large values of the width we find values of $C_{\rm CKM}$ much less than 4, indicating overfitting. We take as ‘‘good’’ fits ones resulting from widths $\sigma_{\rm parameter}$ that yield a $C_{\rm CKM}$ of order 4; an example of such a fit, with $\sigma_{\rm parameter}=0.03$, is given in Table III. This fit, which was attained after 229 iterations to achieve a 1 part in 10^6 change in the cost function in an iteration (we will use this same convergence criterion throughout), had $C_{\rm mass}=0.13$, $C_{\rm CKM}=4.65$, $C_{\rm scnc}=3\times 10^{-4}$, and $C_{\rm parameter}=38.9$, giving a total cost function $C=43.7$. The values of the parameters giving this fit are as follows:

$$\Omega_\phi=71.27, \quad \Omega_\eta=71.27,$$

$$g_\phi^u=0.811, \quad g_\phi^d=0.0201, \quad g_\phi^e=0.00831,$$

$$g_\eta^u=0.00715, \quad g_\eta^d=0.00112, \quad g_\eta^e=0.000371,$$

$$\delta_{1R}=0.00269, \quad \delta_{2R}=0.0340, \quad \delta_{3R}=-0.0367,$$

$$\delta_{1I}=0.00074, \quad \delta_{2I}=0.0027, \quad \delta_{3I}=-0.0034,$$

$$\theta=150.8°,$$

$$[\beta_\phi^u]=\begin{pmatrix} 0.1612 & 0.0477 & 0.0268 \\ 0.0144 & 0.00024 & -0.0133 \\ -0.0442 & -0.0367 & -0.1562 \end{pmatrix},$$

$$[\beta_\phi^d]=\begin{pmatrix} 0.1660 & 0.1589 & 0.0189 \\ 0.0 & 0.0180 & -0.0190 \\ -0.1398 & -0.0189 & -0.1841 \end{pmatrix},$$

$$[\beta_\phi^e]=\begin{pmatrix} 0.1038 & 0.0 & -0.0517 \\ 0.0 & -0.00081 & -0.0375 \\ -0.0366 & -0.00011 & 0.0230 \end{pmatrix}. \tag{54}$$

We see that the largest value of the β asymmetry parameters is 0.184 in magnitude; so the first question we must address is whether this large asymmetry is needed to reproduce the large mixing $s_{12}=0.221$ between the first and second families. To show that this is not the case, we exhibit the result of rerunning the fit, this time omitting the s_{13} and s_{23} terms from the cost function. The result, attained after 137 iterations, has $C_{\rm mass}=0.04$ (that is, the fitted mass values are right on their targets) and $s_{12}=0.221$, so that the Cabibbo mixing is also right on target, but the largest of the β asymmetry parameters has a magnitude of 0.01, a factor of 18 smaller than in the fit of Eq. (54). The values for the unconstrained third family mixings obtained this way are $s_{13}=0.00021$, $s_{23}=0.00072$, much smaller than in the fit of Eq. (54). So we conclude that the large β asymmetry values of Eq. (54) are needed to get correct fits to the third family mixings; the correct value of s_{12} by itself is obtained with β values much smaller in magnitude than s_{12}, in agreement with our observation in Sec. VII that s_{12} is of zeroth order in the asymmetries.

As a second experiment, which gives further insight into why the model requires large asymmetries to fit the third family mixings, we rerun the fit, replacing the targets for both s_{13} and s_{23} by their geometric mean $\simeq 0.011$, with a standard deviation of 0.0015. We find now convergence in 216 iterations, with $C_{\rm mass}=0.02$ (that is, again the fitted mass values are right on their targets), and values for the CKM mixings of $s_{12}=0.221$, $s_{13}=0.0117$, and $s_{23}=0.0101$. For the other components of the cost function we find $C_{\rm CKM}=0.86$, $C_{\rm scnc}=0.9\times 10^{-4}$, and $C_{\rm parameter}=3.5$, for a total of $C=4.4$. As suggested by the small value of $C_{\rm parameter}$, the largest of the β asymmetry parameters now has a magnitude of 0.028, a factor of 6.6 smaller than in the fit of Eq. (54). We conclude from this fit that what requires the large asymmetries in Eq. (54) is splitting s_{23} and s_{13} from a common mean value.

This conclusion can be understood from a simple analytic model, in which the corrections of Appendix C to U_L^f and $U_R^{f\dagger}$ are neglected. Referring to Eq. (42a), let us write $V_{\rm CKM}$ to first order accuracy as

$$V_{\rm CKM}=\begin{pmatrix} 1 & v_{12} \\ -v_{12}^* & 1 \end{pmatrix}, \tag{55a}$$

so that the fitted s_{12} is given by $s_{12}=|v_{12}|$. Then from the approximation of Eq. (42b) for $U_{\rm CKM}$, together with the *CP* invariance condition [see Eq. (38b) and the discussion following Eq. (39c)] $\sigma_{13}^f=\sigma_{23}^{f*}$, we find that

$$s_{13}=|s_3-d_3|/3, \quad s_{23}=|s_3+d_3|/3,$$
$$s_3\equiv\sigma_{13}^u-\sigma_{13}^d, \quad d_3\equiv v_{12}\sigma_{23}^d. \tag{55b}$$

Thus, the spread of s_{13} and s_{23} from their geometric mean is governed by d_3, in which the quantity σ_{23}^d, which is a linear combination of the β asymmetries, is suppressed in magnitude by a factor of $|v_{12}|=s_{12}=0.221$. This is why large β asymmetries are needed to fit the experimental data, whereas much smaller asymmetries suffice when the observed s_{13} and s_{23} are replaced in the fitting program by their geometric mean. For example, in the fit of Eq. (54), the magnitude of d_3 is 0.0445, which corresponds to a value $\sigma_{23}^d=0.0445/0.221=0.20$, similar in size to the maximum β asymmetries found in the fits. Thus, the six-Higgs-doublet model interprets the large difference in magnitude between the observed s_{13} and s_{23} as indicating asymmetries in the Yukawa couplings substantially larger than one might naively infer from the magnitude of s_{23}. The possible relevance of this observation to the extension of our model to neutrino mixing will be discussed in Sec. X.

We next address issues of fine-tuning and naturalness in the six-Higgs-doublet model. In the fit of Eq. (54), the absolute values of the matrix elements of the matrices $U_L^{u,d}$ and $U_R^{d\dagger}$ take the values

$$[|U_L^u|]=\begin{pmatrix} 0.974 & 0.224 & 0.055 \\ 0.224 & 0.974 & 0.034 \\ 0.046 & 0.045 & 1.000 \end{pmatrix}, \tag{56a}$$

$$[|U_L^d|]=\begin{pmatrix} 1.000 & 0.00010 & 0.066 \\ 0.00010 & 1.000 & 0.067 \\ 0.066 & 0.067 & 1.000 \end{pmatrix}, \tag{56b}$$

$$[|U_R^{d\dagger}|]=\begin{pmatrix} 1.000 & 0.00010 & 0.033 \\ 0.00010 & 1.000 & 0.036 \\ 0.033 & 0.036 & 1.000 \end{pmatrix}. \tag{56c}$$

We see that the mixing s_{12} of the first two families arises nearly entirely from U_L^u, while the 2×2 submatrices of U_L^d and $U_R^{d\dagger}$, which mix the first two families (and which are equal to good accuracy), are nearly the unit matrix, which is what allows the strangeness-changing neutral current constraint to be satisfied. To estimate the amount of fine-tuning involved in this, we note that $|D_{\rm Higgs}|$ of Eq. (47b) is quadratic in the matrix element $|U_{L12}^d|\simeq|U_{R12}^{d\dagger}|$. Hence, if the entry for $|D_{\rm Higgs}|/(2.6\times10^{-14})$ in Table III were scaled up from 0.016 to unity, corresponding to the strangeness-changing neutral current constraint being just barely satisfied, the off-diagonal matrix elements $|U_{L12}^d|\simeq|U_{R12}^{d\dagger}|$ in Eqs. (56b), (56c) would be scaled up from 0.00010 to $0.00010/0.016^{1/2}\simeq0.00079$. Taking as a ''generic'' off-diagonal matrix element the average value $\simeq0.05$ of the 13 and 23 matrix elements of Eqs. (56b), (56c), we estimate that fine-tuning in the mixing matrices, of order a factor of $0.05/0.00079\simeq63$, is involved in satisfying the strangeness-changing neutral current constraint, for an assumed Higgs boson mass in the fit [see the second line in Eq. (46b)] of $M_R^{(-)}=(4.5\times0.3)^{1/2}\Omega_\phi\simeq83$ GeV. For a Higgs boson mass of 330 GeV the fine-tuning would be correspondingly reduced to a factor of roughly 16, and for a Higgs boson mass of 800 GeV the fine-tuning factor would be roughly 6.

Given that there is some fine-tuning involved in obeying the strangeness-changing neutral current constraint, one can ask whether it is natural or unnatural to the experimental data. If the fine-tuning is not natural to the data being fit, one would expect the fits to the masses and CKM parameters to improve, or the convergence to a fit to become faster, when the cost function term $C_{\rm scnc}$ is omitted from the total cost function. Performing this experiment, we find that without $C_{\rm scnc}$, a comparably good fit is obtained ($C_{\rm mass}=0.64$, $C_{\rm CKM}=4.1$) as with the cost function term $C_{\rm scnc}$ included, but 600 iterations, as opposed to 229, are required for comparable convergence. In other words, the strangeness-changing neutral current constraint appears to guide the search to a region of parameter space that gives a good fit; we interpret this as an indication that the fine-tuning involved in satisfying this constraint is in fact natural to the data.

One other place where there is fine-tuning in the fits is in the first family masses, since these are naturally zero only in the absence of Yukawa coupling asymmetries. In principle, if the first family cost function terms are omitted from $C_{\rm mass}$, one might expect first family masses as large as 0.2 (the value of the maximum asymmetry parameters) times the corresponding third family masses, which would give $M_u\sim35$, $M_d\sim0.9$, $M_e\sim0.4$. However, performing the experiment of omitting first family mass constraints from the fit, we find first family masses $M_u\simeq0.9$, $M_d\simeq0.23$, $M_e\simeq0.07$; that is, the first family masses are still smaller (or, in the case of M_d, equal to) the second family masses. We interpret this as an indication that small first family masses are in fact natural to the remaining experimental data when first family masses are excluded, in the framework of the six-Higgs-doublet model.

We conclude this section by giving some comparative fits in the three-Higgs-doublet model. Using the same cost function parameters and convergence criterion as in the six-Higgs-doublet case, we get the three-Higgs-doublet model fit shown in Table IV, which required 864 iterations. The mass fit is generally good, except for the low value $M_s=0.037$ (corresponding to $C_{\rm mass}=7.3$), while the CKM parameters

TABLE IV. Three-Higgs-doublet model fit to experimental data.

Quantity	Target value	Fitted value
$v=6^{1/2}\Omega_\phi$	247.0	247.0
M_u	0.005	0.005
M_c	1.30	1.28
M_t	173.0	173.0
M_d	0.010	0.011
M_s	0.200	0.037
M_b	4.30	4.31
M_e	0.00051	0.00051
M_μ	0.1057	0.1057
M_τ	1.777	1.777
$\frac{\lvert D_{\mathrm{Higgs}}\rvert}{2.6\times 10^{-14}}$	0.0	0.001
s_{12}	0.221	0.221
s_{13}	0.0035	0.0037
s_{23}	0.041	0.039
$\lvert\sin\delta_{13}\rvert$	0.60	0.55

are close to their targets ($C_{\mathrm{CKM}}=0.5$). When the strangeness-changing neutral current constraint is omitted in this case, we find faster convergence (398 iterations) and a better fit, with $M_s=0.151$ (corresponding to $C_{\mathrm{mass}}=0.7$) and with the CKM parameters right on target ($C_{\mathrm{CKM}}=0.1$). This behavior contrasts sharply with what we saw in the six-Higgs-doublet model fits, and we interpret it as indicating that the strangeness-changing neutral current constraint is not natural to the data as interpreted in the three-Higgs-doublet model.

X. EXPERIMENTAL ISSUES, NEUTRINO MIXING, COUPLING CONSTANT UNIFICATION, AND DIRECTIONS FOR FUTURE WORK

Of the two models that we have developed in the previous sections, we find the six-Higgs-doublet model the more interesting as a candidate for an extension of the standard model into the energy region that will become accessible in the next decade. As compared with the three-Higgs-doublet model, the six-Higgs-doublet model has fewer parameters, gives better overall fits to the data, and gives some indication that the strangeness-changing neutral current constraint is natural to the data. It also violates *CP* spontaneously in an interesting way that is correlated with the generation of second family masses for the u,d,e families.

The prime experimental signature of the six-Higgs-doublet model is the spectrum of Higgs states tabulated in Table II. If the potential V_2 that couples the ϕ to η Higgs overall phases is in fact small, then the lightest Higgs states should be the pseudo Goldstone bosons. However, because of the $\frac{1}{2}$ power scaling law of Eq. (25c), they need not be so light as to conflict with current Higgs boson mass limits. For example, if the Higgs boson masses M_{Higgs} that enter into the strangeness-changing neutral current constraint are of order 330 GeV, and $V_2/V_{\phi,\eta}\sim 0.1$, which is in the weak coupling regime, then the pseudo Goldstone boson masses are expected to be of order $(0.1)^{1/2}330$ GeV $\simeq 104$ GeV, above current Higgs boson mass limits.

Although we have included the possibility of a right-handed neutrino, and of Dirac neutrino masses and mixing analogous to CKM mixing, in our Lagrangian, we have not attempted a detailed study of the neutrino sector because the experimental picture there is still incomplete. However, let us briefly address the recent report by the Super-Kamiokande Collaboration [16] of evidence for atmospheric neutrino oscillations, suggesting large mixing (of order unity) of second and third family neutrinos. This is clearly a different pattern than is seen for the charged fermion mixings, where, for example, in the fit of Eq. (54) the μ-τ mixing matrix elements of U_L^e are smaller than 0.01 in magnitude. Large ν_μ-ν_τ mixing can be accommodated in our model, nonetheless, by assuming that the Yukawa coupling ratio g_η^f/g_ϕ^f, which we have taken to be small for $f=u,d,e$, is close to unity for $f=\nu$. Together with $\Omega_\eta/\Omega_\phi\simeq 1$, this implies that R^ν of Eq. (39b) is close to unity in magnitude (although it can have a nonzero phase). Referring to Eqs. (38a),(38b), we see that this implies that the neutrino mass matrix is now nearly degenerate in the two-dimensional subspace spanning the second and third families, and so small asymmetries, or asymmetries nearly equal in magnitude, then imply nearly maximal mixing. To show this explicitly, let us apply the analysis of Appendix B to the mass matrix

$$m=\begin{pmatrix} R^\nu & \frac{1}{3}\sigma_{23} \\ \frac{1}{3}\sigma_{32} & 1 \end{pmatrix}. \tag{57a}$$

Then for $M_L=mm^\dagger$, we have, from Eq. (B2b),

$$M_L=\begin{pmatrix} |R^\nu|^2+\frac{1}{9}|\sigma_{23}|^2 & \frac{1}{3}(R^\nu\sigma_{32}^*+\sigma_{23}) \\ \frac{1}{3}(\sigma_{32}R^{\nu *}+\sigma_{23}^*) & 1+\frac{1}{9}|\sigma_{32}|^2 \end{pmatrix}, \tag{57b}$$

and so Eq. (B4b) gives, for the mixing angle,

$$\Theta=\frac{1}{2}\tan^{-1}\left(\frac{-\frac{2}{3}|R^\nu\sigma_{32}^*+\sigma_{23}|}{|R^\nu|^2-1+\frac{1}{9}(|\sigma_{23}|^2-|\sigma_{32}|^2)}\right). \tag{57c}$$

Thus there is maximal mixing whenever

$$\frac{2}{3}|R^\nu\sigma_{32}^*+\sigma_{23}|\gg|R^\nu|^2-1+\frac{1}{9}(|\sigma_{23}|^2-|\sigma_{32}|^2). \tag{57d}$$

If $|R^\nu|$ is close to unity, this inequality can be satisfied either (i) if σ_{23} and σ_{32} are both small or (ii) if the magnitudes of σ_{23} and σ_{32} are not small, but are approximately equal. In

Sec. IX we saw that to reproduce the observed CKM parameters s_{23} and s_{13}, we needed sizable asymmetries (of order 0.2), which if also present in the neutrino sector β's would allow near maximal mixing of the second and third family neutrinos by case (ii) even when the ratio R_ν is only approximately unity in magnitude. Thus large ν_μ-ν_τ mixing is easy to achieve in the six-Higgs-doublet model. Less natural is near degeneracy of the masses of ν_e and ν_μ, as appears to be needed for both the Mikheyev-Smirnov-Wolfenstein (MSW) and the vacuum oscillation interpretations of the solar neutrino data, since the first family masses are zero in our model in the absence of Yukawa asymmetries. Such a degeneracy would have to be the result of sizable asymmetries together with substantial fine-tuning in the neutrino mass matrix, either to raise the ν_e mass to close to the ν_μ mass in case (i) or to lower the ν_μ mass to close to zero in case (ii) (as, for example, is done in the model of Barger *et al.* [17]; see also Baltz, Goldhaber, and Goldhaber [17]). In either case, there will almost certainly be large mixing of ν_e with ν_μ; so on this (very preliminary) interpretation, our model would favor the large angle as opposed to the small angle MSW solution.

Let us next address the issue of coupling constant unification in the six-Higgs-doublet model. Because we do not alter the fermion representation content of the standard model, the usual running coupling analysis applies. As noted by Langacker [18], the standard model with $\simeq 7$ (by current data [19], 7.66) Higgs boson doublets gives one-loop coupling constant unification with a unification energy of order 5×10^{13} GeV. Even with only six Higgs doublets, the magnitude of two-loop radiative corrections [20] is sufficient to make coupling constant unification a possibility. Of course, because the unification energy is lower than in the customary scenario, a mechanism is needed to suppress proton decay, such as is present in the SU(15) family [21] of grand unification models. Clearly, definitive statements here will depend on the nature of the high energy theory for which the six-Higgs-doublet model is a low energy effective theory; the point we wish to stress, though, is that the six-Higgs-doublet model may be a candidate for coupling constant unification without the assumption of low energy supersymmetry. Whether such a candidate is needed, of course, will depend on the outcome of supersymmetry searches over the next decade.

There are a number of obvious directions for further work on the models we have developed in this paper. Entirely within the low energy effective action framework, one can address the issue of one-loop radiative corrections to the mass and mixing matrix analysis given here. This will involve the parameters determining the Higgs boson masses in an integral way, and if the six-Higgs-doublet model is to be viable, the one-loop corrections should improve, rather than make worse, the comparisons with experiment and the consistency tests discussed in Sec. IX. Another issue that can be addressed within the low energy framework is the magnitude of electroweak baryogenesis in the six-Higgs-doublet model and cosmological implications of this model more generally. At a deeper level, there is the issue of finding a grand unified model, composite model, or hybrid model comprising elements of both, which is a natural high energy physics source for the low energy effective action physics described by the six-Higgs-doublet model. Such a high energy model must, through its representation content and instanton physics, justify the discrete chiral transformation rules assumed in Eqs. (1a)–(1c), and it is also the place where one must seek explanations for the ''vertical'' hierarchy of Yukawa coupling strengths and the pattern of Yukawa coupling asymmetries, which is needed for our fits.

Added note. After this paper was posted to the Los Alamos e-print archive, two earlier papers that use families of Higgs scalars (although without the ingredient of Z_6 discrete chiral symmetry analyzed here) were brought to my attention. The paper of Derman and Jones [22] studies a two-family, two-Higgs-doublet model with an S_2 permutation symmetry, and is probably the earliest paper to extend the idea of family symmetries to the Higgs sector; the paper of Derman [23] extends this to three families of fermions and Higgs doublets with an S_3 permutation symmetry.

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APPENDIX A: NUMERICAL MINIMIZATION OF THE HIGGS POTENTIAL

Because the Higgs potential of Eqs. (7a)–(7c) is complicated, even with the simplifying assumptions of *CP* invariance and cyclic permutation symmetry, we have supplemented our analytic studies of the Higgs extrema with numerical studies, performed by using the conjugate gradient method to minimize the Higgs potential. Since it is easy to analytically compute the first derivatives (the gradients) of the Higgs potential, it is advantageous to use the conjugate gradient method in a form where both the function to be minimized and its derivatives are externally supplied; this gives a faster routine and there is some built-in redundancy that serves as a check, since the same information is in effect furnished twice, once through the computation of the function and a second time through the independent computation of its derivatives. We have used the minimization program FRPRMN of Press *et al.* [12], with the following modification. Press *et al.* base the convergence criterion in their program on computing the change in the *function value* over one iteration, but this results in significant truncation error inaccuracies for the minimizing values of the *arguments* (the Higgs fields) when the function is large in magnitude but very flat at its minimum. Since the gradients are explicitly known, and since at the minimum the gradients must all vanish, much better accuracy for the minimizing Higgs fields is obtained by making the convergence criterion depend on the maximum gradient. With this modification to FRPRMN, one can verify the vanishing of the gradients to double precision accuracy at the Higgs potential minimum.

To obtain the formulas for the gradients, as a function of general ϕ,η, we substitute $\phi\to\phi+\delta\phi,\eta\to\eta+\delta\eta$ into Eqs. (7a)–(7c), and retain the first order variations, which can be brought to the convenient form

$$\delta\mathcal{L}_{\text{Higgs potential}}=\text{Re}\sum_{n=1}^{3}(C_n^{\phi}\delta\phi_n^*+C_n^{\eta}\delta\eta_n^*). \quad \text{(A1a)}$$

We assume both CP invariance and cyclic permutation symmetry; using the latter we get formulas for $C_{2,3}^{\phi,\eta}$ by cyclic permutation of the arguments of $C_1^{\phi,\eta}$. Changing notation for the coefficients from C_{lmn} to $C_{l;mn}$, to avoid notational ambiguities when explicit numerical values are assigned for m, we obtain the following explicit expressions for $C_1^{\phi,\eta}$:

$$\begin{aligned}C_1^{\phi}={}&4\lambda_{\phi}(\phi_1^*\phi_1-v_{\phi}^2)\phi_1-2(\mu_{1\phi}+\mu_{2\phi})(\phi_2^*\phi_2+\phi_3^*\phi_3)\phi_1-\alpha_{\phi}(2\phi_2\phi_1^*\phi_3+\phi_3^2\phi_2^*+\phi_2^2\phi_3^*)+\gamma\eta_1\\&+\sum_{m=1}^{3}[2C_{1;1m}\eta_m^*\eta_m\phi_1+C_{2;1m}\eta_1\eta_m^*\phi_m+C_{2;m1}\eta_1\eta_m^*\phi_m+C_{3;1m}\phi_2\eta_m^*\eta_{m-1}+C_{3;3m}\phi_3\eta_{m-1}^*\eta_m+C_{4;m1}\phi_3\eta_m^*\eta_{m+1}\\&+C_{4;m2}\phi_2\eta_m\eta_{m+1}^*+C_{5;1m}\eta_2\eta_m^*\phi_{m-1}+C_{5;m2}\eta_2\eta_{m+1}^*\phi_m+C_{6;m1}\eta_3\eta_m^*\phi_{m+1}+C_{6;3m}\eta_3\eta_{m-1}^*\phi_m+C_{7;1m}\phi_2\phi_m^*\eta_{m-1}\\&+C_{7;3m}\phi_3\phi_m\eta_{m-1}^*+C_{7;m1}\phi_m^*\phi_{m+1}\eta_3+C_{8;1m}\phi_2\eta_m^*\phi_{m-1}+C_{8;3m}\phi_3\eta_m\phi_{m-1}^*+C_{8;m2}\phi_m\phi_{m+1}^*\eta_2+C_{9;m1}\eta_m^*\eta_{m+1}\eta_3\\&+C_{10;m2}\eta_m\eta_{m+1}^*\eta_2+C_{11;1m}\eta_2\phi_m^*\eta_{m-1}+C_{11;m1}\phi_m^*\eta_{m+1}\eta_3+C_{12;3m}\eta_3\eta_m\phi_{m-1}^*+C_{12;m2}\eta_m\phi_{m+1}^*\eta_2],\end{aligned} \quad \text{(A1b)}$$

$$\begin{aligned}C_1^{\eta}={}&4\lambda_{\eta}(\eta_1^*\eta_1-v_{\eta}^2)\eta_1-2(\mu_{1\eta}+\mu_{2\eta})(\eta_2^*\eta_2+\eta_3^*\eta_3)\eta_1-\alpha_{\eta}(2\eta_2\eta_1^*\eta_3+\eta_3^2\eta_2^*+\eta_2^2\eta_3^*)+\gamma\phi_1+\sum_{m=1}^{3}[2C_{1;m1}\phi_m^*\phi_m\eta_1\\&+C_{2;m1}\phi_1\phi_m^*\eta_m+C_{2;1m}\phi_1\phi_m^*\eta_m+C_{3;m1}\eta_3\phi_m^*\phi_{m+1}+C_{3;m2}\eta_2\phi_m\phi_{m+1}^*+C_{4;1m}\eta_2\phi_m^*\phi_{m-1}+C_{4;3m}\eta_3\phi_m\phi_{m-1}^*\\&+C_{5;m1}\phi_3\phi_m^*\eta_{m+1}+C_{5;3m}\phi_3\phi_{m-1}^*\eta_m+C_{6;1m}\phi_2\phi_m^*\eta_{m-1}+C_{6;m2}\phi_2\phi_{m+1}^*\eta_m+C_{7;m2}\phi_m\phi_{m+1}^*\phi_2+C_{8;m1}\phi_m^*\phi_{m+1}\phi_3\\&+C_{9;1m}\eta_2\phi_m^*\eta_{m-1}+C_{9;3m}\eta_3\phi_m\eta_{m-1}^*+C_{9;m2}\eta_m\eta_{m+1}^*\phi_2+C_{10;1m}\eta_2\eta_m^*\phi_{m-1}+C_{10;3m}\eta_3\eta_m\phi_{m-1}^*\\&+C_{10;m1}\eta_m^*\eta_{m+1}\phi_3+C_{11;3m}\phi_3\phi_m\eta_{m-1}^*+C_{11;m2}\phi_m\eta_{m+1}^*\phi_2+C_{12;1m}\phi_2\eta_m^*\phi_{m-1}+C_{12;m1}\eta_m^*\phi_{m+1}\phi_3].\end{aligned} \quad \text{(A1c)}$$

APPENDIX B: BI-UNITARY DIAGONALIZATION OF A 2×2 MATRIX

We give here the method for constructing the matrices V_L and $V_R^{\dagger}$ that obey Eq. (41a) of the text, suppressing the flavor index f throughout. Let m by the 2×2 complex matrix defined by

$$m=\begin{pmatrix}\sigma_{11} & \sigma_{12}\\ \sigma_{21} & \sigma_{22}\end{pmatrix}. \quad \text{(B1)}$$

We begin by forming the self-adjoint matrices $M_L\equiv mm^{\dagger}$ and $M_R\equiv m^{\dagger}m$, which we write in the form

$$M_L=\begin{pmatrix}A_L & z_L^*\\ z_L & B_L\end{pmatrix},\quad M_R=\begin{pmatrix}A_R & z_R^*\\ z_R & B_R\end{pmatrix}, \quad \text{(B2a)}$$

with

$$A_L=|\sigma_{11}|^2+|\sigma_{12}|^2,$$

$$B_L=|\sigma_{21}|^2+|\sigma_{22}|^2,$$

$$z_L=\sigma_{11}^*\sigma_{21}+\sigma_{12}^*\sigma_{22} \quad \text{(B2b)}$$

and

$$A_R=|\sigma_{11}|^2+|\sigma_{21}|^2,$$

$$B_R=|\sigma_{12}|^2+|\sigma_{22}|^2,$$

$$z_R=\sigma_{12}^*\sigma_{11}+\sigma_{22}^*\sigma_{21}. \quad \text{(B2c)}$$

The quantities just defined are not independent, since it is easy to verify that

$$A_L+B_L=A_R+B_R,$$

$$\frac{1}{4}(A_L-B_L)^2+|z_L|^2=\frac{1}{4}(A_R-B_R)^2+|z_R|^2,$$

$$|z_L|^2\leqslant A_LB_L,\quad |z_R|^2\leqslant A_RB_R. \quad \text{(B2d)}$$

The desired bi-unitary matrices will be the V_L for which $V_LM_LV_L^{\dagger}$ is diagonal, and the V_R for which $V_RM_RV_R^{\dagger}$ is diagonal, with eigenvalues ordered in magnitude.

Thus, defining the self-adjoint matrix M by

$$M=\begin{pmatrix} A & z^* \\ z & B \end{pmatrix}, \quad |z|^2 \leqslant AB, \tag{B3a}$$

it suffices to find the diagonalizing unitary transformation V that yields

$$VMV^\dagger=\begin{pmatrix} |\kappa_1|^2 & 0 \\ 0 & |\kappa_2|^2 \end{pmatrix}, \quad |\kappa_1|\leqslant|\kappa_2|; \tag{B3b}$$

then all that we have to do is to apply this construction twice, first to M_L and then to M_R. Let us write M in Pauli matrix form as

$$M=\frac{1}{2}(A+B)+\vec{v}\cdot\vec{\tau}, \quad \vec{v}=\left(z_R, z_I, \frac{1}{2}(A-B)\right), \tag{B3c}$$

with $z_{R,I}$ the real and imaginary parts of z. Representing the diagonalizing V in Pauli matrix form as

$$V=\exp(i\Theta\vec{n}\cdot\vec{\tau})=\cos\Theta+i\vec{n}\cdot\vec{\tau}\sin\Theta, \tag{B4a}$$

and letting $\hat{z}=(0,0,1)$ be the unit vector in the third axis direction, a simple calculation shows that we satisfy Eq. (B3b) by taking

$$\begin{aligned}
\sin 2\Theta &= \frac{|\hat{z}\times\vec{v}|}{|\vec{v}|}=\frac{|z|}{[\frac{1}{4}(A-B)^2+|z|^2]^{1/2}}, \\
\cos 2\Theta &= \frac{-\hat{z}\cdot\vec{v}}{|\vec{v}|}=\frac{-\frac{1}{2}(A-B)}{[\frac{1}{4}(A-B)^2+|z|^2]^{1/2}}, \\
\Theta &= \frac{1}{2}\tan^{-1}\left(\frac{-2|z|}{A-B}\right), \\
\hat{n} &= -\frac{\hat{z}\times\vec{v}}{|\hat{z}\times\vec{v}|}=\frac{(z_I, -z_R, 0)}{|z|},
\end{aligned} \tag{B4b}$$

and that this V gives

$$VMV^\dagger=\frac{1}{2}(A+B)-|\vec{v}\,|\tau_3. \tag{B4c}$$

Thus we see that the squared eigenvalues are

$$|\kappa_1|^2=\frac{1}{2}(A+B)-|\vec{v}|, \quad |\kappa_2|^2=\tfrac{1}{2}(A+B)+|\vec{v}\,|, \tag{B5a}$$

which are correctly ordered; the smaller squared eigenvalue is guaranteed to be non-negative by virtue of the fact that the product of the squared eigenvalues is

$$\tfrac{1}{4}(A+B)^2-|\vec{v}\,|^2=AB-|z|^2\geqslant 0. \tag{B5b}$$

When $|z|=0$, the above formulas are indeterminate; we then get the correct eigenvalue ordering by taking $\sin 2\Theta=0$ and $\cos 2\Theta=\pm 1$, with the $+$ sign holding for $A\leqslant B$ and the $-$ sign holding for $A>B$. Referring back to the identities of Eq. (B2d), we see that they imply that $|\vec{v}_L|=|\vec{v}_R|$, and thus the eigenvalues are the same for M_L and M_R, as expected. Substituting the expression for $\hat{n}$ in Eq. (B4b) back into Eq. (B4a), we get the further useful expression

$$V=\begin{pmatrix} \cos\Theta & -\dfrac{z^*}{|z|}\sin\Theta \\ \dfrac{z}{|z|}\sin\Theta & \cos\Theta \end{pmatrix}. \tag{B6}$$

APPENDIX C: IMPROVED FORMULAS FOR U_L^f AND $U_R^{f\dagger}$

In our numerical work, we used an improved approximation to U_L^f and $U_R^{f\dagger}$ obtained by adding to Eqs. (41b), (41c) the respective corrections ΔU_L^f and $\Delta U_R^{f\dagger}$, given by

$$\Delta U_L^f=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{9}\kappa_2^f\eta_{32}^{f*} \\ \frac{1}{9}\kappa_2^{f*}\eta_{32}^f V_{L21}^f & \frac{1}{9}\kappa_2^{f*}\eta_{32}^f V_{L22}^f & 0 \end{pmatrix} \tag{C1a}$$

and

$$\Delta U_R^{f\dagger}=\begin{pmatrix} 0 & 0 & \frac{1}{9}V_{R12}^{f\dagger}\kappa_2^{f*}\eta_{23}^f \\ 0 & 0 & \frac{1}{9}V_{R22}^{f\dagger}\kappa_2^{f*}\eta_{23}^f \\ 0 & -\frac{1}{9}\kappa_2^f\eta_{23}^{f*} & 0 \end{pmatrix}. \tag{C1b}$$

Here $V_{L,R}^f$ are the matrices defined in Eq. (41a) and computed in Appendix B, κ_2^f is the eigenvalue defined in Eq. (41a), given explicitly by

$$\begin{aligned}\kappa_2^f={}&V_{L21}^f(\sigma_{11}^f V_{R12}^{f\dagger}+\sigma_{12}^f V_{R22}^{f\dagger})+V_{L22}^f(\sigma_{21}^f V_{R12}^{f\dagger} \\ &+\sigma_{22}^f V_{R22}^{f\dagger}),\end{aligned} \tag{C2a}$$

and the quantities η_{23}^f, η_{32}^f are defined by

$$\begin{aligned}\eta_{23}^f&=V_{L21}^f\sigma_{13}^f+V_{L22}^f\sigma_{23}^f, \\ \eta_{32}^f&=\sigma_{31}^f V_{R12}^{f\dagger}+\sigma_{32}^f V_{R22}^{f\dagger}.\end{aligned} \tag{C2b}$$

These corrections make the formulas for U_L^f and $U_R^{f\dagger}$ accurate to first order when $(|\kappa_2^f|/3)^2$, rather than $|\kappa_2^f|/3$, is regarded as a first order small quantity. They have only a small effect on the fits of Sec. IX (because for charged fermions the second to third generation mass ratios are small), but are useful in performing accurate numerical checks that $U_L^f M_f' U_R^{f\dagger}$ is diagonal.

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