Symmetries of two Higgs doublet model and *CP* violation

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We use the invariance of a physical picture under a change of Lagrangian, the reparameterization invariance in the space of Lagrangians and its particular case—the rephrasing invariance—for analysis of the two-Higgs-doublet extension of the standard model. We found that some parameters of theory like $\tan\beta$ are reparameterization dependent and therefore cannot be fundamental. We use the Z_2 symmetry of the Lagrangian, which prevents a $\phi_1 \leftrightarrow \phi_2$ transition, and the different levels of its violation, soft and hard, to describe the physical content of the model. In general, the broken Z_2 symmetry allows for a *CP* violation in the physical Higgs sector. We argue that the two-Higgs-doublet model with a soft breaking of Z_2 symmetry is a natural model in the description of electroweak symmetry breaking. To simplify the analysis, we choose among different forms of Lagrangian describing the same physical reality a specific one, in which the vacuum expectation values of both Higgs fields are real. A possible *CP* violation in the Higgs sector is described by using a two-step procedure with the first step identical to a diagonalization of the mass matrix for *CP*-even fields in the *CP*-conserving case. We find a very simple, necessary, and sufficient condition for a *CP* violation in the Higgs sector. We determine the range of parameters for which *CP* violation and flavor-changing neutral current effects are naturally small—it corresponds to a small dimensionless mass parameter $\nu = \mathrm{Re}m_{12}^2/(2v_1v_2)$. We show that for small ν some Higgs bosons can be heavy—with mass up to about 0.6 TeV—without violating of the unitarity constraints. If ν is large, all Higgs bosons except one can be arbitrarily heavy. We discuss, in particular, main features of this case, which corresponds for $\nu \to \infty$ to a decoupling of heavy Higgs bosons. In the model II for Yukawa interactions we obtain the set of relations among the couplings to gauge bosons and to fermions which allows us to analyze different physical situations (including *CP* violation) in terms of these very couplings, instead of the parameters of Lagrangian.

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I. INTRODUCTION

A spontaneous electroweak symmetry breaking of $SU(2)\times U(1)$ (EWSB) via the Higgs mechanism is described by the Lagrangian

$$\mathcal{L} = \mathcal{L}_{gf}^{\mathrm{SM}} + \mathcal{L}_H + \mathcal{L}_Y. \tag{1.1}$$

Here, $\mathcal{L}_{gf}^{\mathrm{SM}}$ describes the $SU(2)\times U(1)$ standard model interaction of gauge bosons and fermions, $\mathcal{L}_H$ is the Higgs scalar Lagrangian, and $\mathcal{L}_Y$ describes the Yukawa interactions of fermions with Higgs scalars.

In the minimal standard model (SM) one scalar isodoublet with hypercharge $Y = 1$ is implemented. Here $\mathcal{L}_H = (D_\mu\phi)^\dagger D_\mu\phi - V$, with the Higgs potential $V = \lambda\phi^4/2 - m^2\phi^2/2$. A minimum of V describes the vacuum expectation value (v.e.v.) v as $\langle\phi\rangle = v/\sqrt{2} = \sqrt{m^2/2\lambda}$. In this model there is one physical Higgs boson; its couplings to the gauge bosons can be expressed via masses as $g_W^{\mathrm{SM}} = \sqrt{2}M_W/v$, $g_Z^{\mathrm{SM}} = \sqrt{2}M_Z/v$. The Yukawa interaction has a form:

$$\mathcal{L}_Y = \sum g_f^{\mathrm{SM}}\overline{Q}_L\phi q_R + \mathrm{H.c.} \quad \text{with } g_f^{\mathrm{SM}} = \sqrt{2}m_f/v.$$

In this paper we study in detail the simplest extension of the SM, with one extra scalar doublet called the two-Higgs-doublet model (2HDM) which contains more physical neutral and charged Higgs bosons (see e.g. [1]). We treat a *CP* violation in the Higgs sector as a natural feature of the theory.

This model contains two doublet fields, ϕ_1 and ϕ_2, with identical quantum numbers. Therefore, its most general form should allow for global transformations which mix these fields and change the relative phase. Each such transformation generates a new Lagrangian, with parameters given by parameters of the incident Lagrangian and parameters of the transformation. That is *the reparameterization transformation*[1] of parameters of the Lagrangian. Therefore, the physical reality described by some Lagrangian $\mathcal{L}$ (*physical model*) is also described by many other Lagrangians. We call this property *a reparameterization invariance* in *a space of Lagrangians (with coordinates given by its parameters)* and discuss it together with its particular case—*a rephasing invariance*—in Sec. II A.

If a given Lagrangian demonstrates some property, say AAA, explicitly, we call it *the AAA Lagrangian or the Lagrangian of AAA form*; a set of reparameterization equivalent Lagrangians with the same explicit property constitutes *a AAA family of Lagrangians*.

[1]This very transformation is called in [2] as Higgs basis transformation.

We found that some quantities, considered often as fundamental parameters of theory, like $\tan\beta$—a ratio of vacuum expectation values of fields ϕ_1 and ϕ_2—are in fact reparameterization dependent.

One of the earliest reasons for introducing the 2HDM was to describe the phenomenon of CP violation [3], an effect which can be potentially large. Glashow and Weinberg [4] found that the CP violation and the flavor-changing neutral currents (FCNC) can be naturally suppressed by imposing on the Lagrangian a Z_2 symmetry, that is the invariance on the Lagrangian under the interchange

$$\phi_1 \leftrightarrow \phi_1, \qquad \phi_2 \leftrightarrow -\phi_2 \quad \text{or} \\ \phi_1 \leftrightarrow -\phi_1, \qquad \phi_2 \leftrightarrow \phi_2. \tag{1.2}$$

This symmetry forbids the $\phi_1 \leftrightarrow \phi_2$ transitions.

The most general Yukawa interaction $\mathcal{L}_Y$ violates this Z_2 symmetry leading to the potentially large flavor-changing neutral current effects. The Yukawa interaction can lead (via loop corrections) to the CP violation even if such violation is absent in the basic Higgs Lagrangian. Imposing some constraints on $\mathcal{L}_Y$ allows to eliminate this source of the CP violation.

Since in nature both the CP violation and FCNC effects are small, we discuss separately cases of the exact Z_2 symmetry (then CP is conserved) and of different levels of its violation, soft and hard. We consider also a general renormalizability of widely discussed forms of 2HDM Lagrangians. We analyze these problems in Sec. II B.

The EWSB is described by vacuum expectation values of fields $\phi_{1,2}$ with generally different phases. This phase difference can be eliminated by a suitable rephasing transformation, resulting in the *Lagrangian in a real vacuum form* (see Sec. III). We use such a Lagrangian in a particular form with coefficients of the mass (quadratic) terms in the Higgs potential expressed by coefficients of quartic terms of potential and vacuum expectation values.

In such form of Lagrangian the real and imaginary parts of a coefficient at the mixed quadratic term, describing a soft violation of Z_2 symmetry, have different properties. The real part can be treated as a free parameter of theory, while the imaginary part (describing a CP violation) is constrained by the parameters of quartic terms of Higgs Lagrangian and the vacuum expectation values.

In Sec. IV we come forward to the observable (physical) Higgs particles. The Goldstone modes and charged Higgs bosons $H^\pm$ are separated easily. In the neutral sector two isotopic doublets give after EWSB one Goldstone mode, two pure scalars (CP-even) η_1, η_2, and one CP-odd "pseudoscalar" A. These three states do generally mix leading to the physical states $h_i (i = 1, 2, 3)$ without a definite CP parity. The interaction of these states with matter gives observable effects of CP violation. We construct these states by a two-step procedure, with the first step corresponding to the diagonalization of a partial mass-squared matrix for CP-even neural components of Higgs doublets. This leads to the states h and H, discussed usually in a context of the CP-conserving case. It allows us to consider a general CP nonconserving case in terms of states h, H, and A, customary in the case of CP conservation. In these terms analyses of CP violation effects become very transparent and some important results can be obtained easily.

In Sec. V the description of Yukawa couplings is given. A most general form of Yukawa interaction violates CP symmetry, leads to a tree-level FCNC, and breaks Z_2 symmetry in a hard way (by loop corrections). A specific form of Yukawa interaction, in which each right-handed fermion isosinglet is coupled to only one scalar field, ϕ_1 or ϕ_2, guarantees an absence of the hard violation of Z_2 symmetry if this violation is absent in the proper Higgs Lagrangian $\mathcal{L}_H$. With such Yukawa sector the CP violation arises only from a structure of the Higgs Lagrangian, and FCNC effects can be naturally small. Here we consider the well-known model II [1] in the explicit form, which is defined with accuracy up to the rephasing transformation.

In the investigation of phenomenological aspects of 2HDM it is useful to apply *relative couplings*, defined as ratios of the couplings of each neutral Higgs boson $h_i (i = 1, 2, 3)$, to the gauge bosons W or Z and to the quarks or leptons ($j = W, Z, u, d, \ell \dots$), to the corresponding SM couplings:

$$\chi_j^{(i)} = g_j^{(i)}/g_j^{\rm SM}. \tag{1.3}$$

As their squared values are in principle measurable, we treat $\chi_j^{(i)}$ themselves as measurable quantities. These relative couplings and the relations among them are less affected by the radiative corrections than the Higgs couplings themselves (see Sec. V D).

We present formulas for the relative couplings describing interactions of the observable Higgs bosons with fermions and gauge bosons and then derive the set of relations among these couplings, including obtained by us *pattern and linear relations* as well as known *sum rules*. These relations are very useful in the analyses of different physical scenarios.

Parameters of Lagrangian are constrained by positivity (vacuum stability) and minimum constraints, discussed in Sec. VI. In most cases the physical phenomena related to the Higgs sector are described with a good accuracy by the lowest nontrivial order of the perturbation theory (that is the tree approximation for the description of the Higgs sector itself and the one-loop approximation for the Yukawa contribution to the Higgs boson propagators and Higgs couplings to the photons and gluons). This should be reliable for not too large values of parameters of quartic terms of the Lagrangian; we consider the relevant *unitarity and perturbativity constraints* in Sec. VI C. Most of the above constraints were obtained in literature for a soft violation of Z_2 symmetry. We discuss the main new aspects in case of the hard violation of Z_2 symmetry in Sec. VI D.

In 2HDM there is an attractive possibility that one of neutral Higgs bosons h_1 is relatively light and similar to that in the SM while others (h_2, h_3, and $H^\pm$) are much heavier; this is discussed in Sec. VII. The studies of 2HDM are based often on an assumption of *decoupling* of these heavy Higgs bosons from the known particles, i.e. effects of these additional Higgs bosons disappear if their masses tend to infinity. However, such an assumption is not necessary for the description of phenomena in the presence of heavy but not extremely heavy new particles.

For the Higgs Lagrangian in a real vacuum form the mentioned decoupling phenomenon is governed by a singe dimensionless parameter $\nu \propto \mathrm{Re} m_{12}^2$. The mass range of possible heavy Higgs bosons, allowed by perturbativity and unitarity constraints, depends strongly on ν. For large ν the decoupling limit is realized, i.e. the above mentioned additional Higgs bosons can be very heavy (and almost degenerate in masses) and moreover such additional Higgs bosons practically decouple from the lighter particles. We analyze briefly properties of all Higgs bosons and their interactions in this decoupling limit.

At small ν masses of h_2, h_3, and $H^\pm$ are bounded from above by the unitarity constraints. Such Higgs bosons can be heavy enough to avoid observation even at next generation of colliders. Nevertheless, some nondecoupling effects can appear for the lightest Higgs boson. We present some sets of parameters which realize this physical picture without decoupling, still respecting the unitarity constraints. We argue that this nondecoupling option of 2HDM is more *natural* for the weak *CP* violation and FCNC (in spirit of t' Hooft's concept of naturalness [5]).

Section VII contains our summary and discussion of results.

In the Appendix we present trilinear and quartic couplings of physical Higgs bosons in a general *CP*-violating case and give the series of useful forms for a full collection of trilinear Higgs self-couplings in the *CP*-conserving, soft Z_2-violating case. For the case when the Yukawa interaction is described by model II, we express all these trilinear couplings via the parameter ν—the masses and the relative couplings to the gauge bosons and fermions of the physical Higgs bosons entering the corresponding vertex.

II. HIGGS LAGRANGIAN

To keep the value of $\rho = M_W^2/(M_Z^2 \cos^2\theta_W)$ equal to 1 at the tree level, one assumes in 2HDM that both scalar fields (ϕ_1 and ϕ_2) are weak isodoublets ($T = 1/2$) with hypercharges $Y = \pm 1$ [6]. We use $Y = +1$ for both doublets (the other choice, $Y_1 = 1$, $Y_2 = -1$, is used in the minimal supersymmetry model (MSSM); this case is also described by equations below with a trivial change of variables).

The most general renormalizable Higgs Lagrangian can be written as

$$\mathcal{L}_H = T - V, \tag{2.1a}$$

where T is the kinetic term with D_μ being the covariant derivative containing the EW gauge fields, and V is the Higgs potential. For 2HDM we have

$$T = (D_\mu \phi_1)^\dagger (D^\mu \phi_1) + (D_\mu \phi_2)^\dagger (D^\mu \phi_2) + \varkappa (D_\mu \phi_1)^\dagger (D^\mu \phi_2) + \varkappa^* (D_\mu \phi_2)^\dagger (D^\mu \phi_1), \tag{2.1b}$$

$$V = \frac{\lambda_1}{2}(\phi_1^\dagger \phi_1)^2 + \frac{\lambda_2}{2}(\phi_2^\dagger \phi_2)^2 + \lambda_3 (\phi_1^\dagger \phi_1)(\phi_2^\dagger \phi_2) + \lambda_4 (\phi_1^\dagger \phi_2)(\phi_2^\dagger \phi_1) + \frac{1}{2}[\lambda_5 (\phi_1^\dagger \phi_2)^2 + \mathrm{H.c.}] + \{[\lambda_6 (\phi_1^\dagger \phi_1) + \lambda_7 (\phi_2^\dagger \phi_2)](\phi_1^\dagger \phi_2) + \mathrm{H.c.}\} \tag{2.1c}$$

$$-\frac{1}{2}\{m_{11}^2 (\phi_1^\dagger \phi_1) + m_{22}^2 (\phi_2^\dagger \phi_2) + [m_{12}^2 (\phi_1^\dagger \phi_2) + \mathrm{H.c.}]\}. \tag{2.1d}$$

The Eq. (2.1d) represents a mass term. Note that λ_{1-4}, m_{11}^2, and m_{22}^2 are real (by Hermiticity of the potential), while the λ_{5-7}, m_{12}^2, and $\varkappa$ are in general complex parameters. (We explain necessity of mixed kinetic $\varkappa$ terms in Sec. II B 2.) Therefore, this potential contains 14 independent parameters while the entire Higgs Lagrangian—16. We will see that *CP* violation in the Higgs sector, which is a natural feature of 2HDM, can appear only if some of these coefficients are complex.

A. Reparameterization and rephasing invariance

1. Reparameterization invariance

Our model contains two fields with identical quantum numbers. Therefore, it can be described both in terms of fields ϕ_k ($k = 1, 2$), used in Lagrangian (2.1), and in terms of fields ϕ_k' obtained from ϕ_k by a global unitary transformation $\hat{\mathcal{F}}$ of the form:

$$\begin{pmatrix} \phi_1' \\ \phi_2' \end{pmatrix} = \hat{\mathcal{F}} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix},$$
$$\hat{\mathcal{F}} = e^{-i\rho_0} \begin{pmatrix} \cos\theta e^{i\rho/2} & \sin\theta e^{i(\tau-\rho/2)} \\ -\sin\theta e^{-i(\tau-\rho/2)} & \cos\theta e^{-i\rho/2} \end{pmatrix}. \tag{2.2}$$

The transformation (2.2) induces the changes of coefficients of Lagrangian, which we call *a reparameterization transformation (RPaT)*. The set of RPaT's represents the 3-parametrical *reparameterization transformation* $SU(2)$ *group*, with *three reparameterization parameters*[2] (ρ, θ, τ) acting in the *16-dimensional space of Lagrangians* with coordinates given by λ_{1-4}, $\mathrm{Re}\lambda_{5-7}$, $\mathrm{Im}\lambda_{5-7}$, $m_{11,22}^2$, $\mathrm{Re}(m_{12}^2)$, $\mathrm{Im}(m_{12}^2)$, $\mathrm{Re}\varkappa$, and $\mathrm{Im}\varkappa$.

[2]Similar to *the gauge parameter* of gauge theories.

In the $\varkappa = 0$ case the transformation (2.2) does not change the form of kinetic term. It induces RPaT's of the form

$$\begin{aligned}
\lambda_1' &= c^2\lambda_1 + s^2\lambda_2 - cs\Phi - 2cs\,\mathrm{Re}(\tilde{\lambda}_6 + \tilde{\lambda}_7),\\
\lambda_2' &= s^2\lambda_1 + c^2\lambda_2 - cs\Phi + 2cs\,\mathrm{Re}(\tilde{\lambda}_6 + \tilde{\lambda}_7),\\
\lambda_3' &= \lambda_3 + cs\Phi, \qquad \lambda_4' = \lambda_4 + cs\Phi,\\
e^{2i\rho}\lambda_5' &= \lambda_5 + e^{i\tau}s[c\Phi + 2is\,\mathrm{Im}\tilde{\lambda}_5 - 2ic\,\mathrm{Im}(\tilde{\lambda}_6 - \tilde{\lambda}_7)],\\
e^{i\rho}\lambda_6' &= c^2\lambda_6 - s^2\lambda_7 + \frac{e^{i\tau}}{2}cs(\lambda_1 - \lambda_2 + \Psi),\\
e^{i\rho}\lambda_7' &= c^2\lambda_7 - s^2\lambda_6 + \frac{e^{i\tau}}{2}cs(\lambda_1 - \lambda_2 - \Psi),
\end{aligned} \tag{2.3a}$$

$$\begin{aligned}
(m')^2_{11} &= c^2 m^2_{11} + s^2 m^2_{22} - 2cs\mu^2_{12},\\
(m')^2_{22} &= s^2 m^2_{11} + c^2 m^2_{22} + 2cs\mu^2_{12},\\
e^{i\rho}(m')^2_{12} &= m^2_{12} + e^{i\tau}[cs(m^2_{11} - m^2_{22}) - 2s^2\mu^2_{12}].
\end{aligned} \tag{2.3b}$$

where $c = \cos\theta$, $s = \sin\theta$, $\mu^2_{12} = \mathrm{Re}(m^2_{12}e^{-i\tau})$, $\tilde{\lambda}_5 = \lambda_5 e^{-2i\tau}$, $\tilde{\lambda}_{6,7} = \lambda_{6,7}e^{-i\tau}$, and

$$\begin{aligned}
&\Phi_0 = \lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4 + \mathrm{Re}\tilde{\lambda}_5),\\
&\Phi = cs\Phi_0 + 2(c^2 - s^2)\,\mathrm{Re}(\tilde{\lambda}_6 - \tilde{\lambda}_7),\\
&\Psi = (c^2 - s^2)\Phi_0 - 8cs\,\mathrm{Re}(\tilde{\lambda}_6 - \tilde{\lambda}_7) + 2i\,\mathrm{Im}\tilde{\lambda}_5.
\end{aligned}$$

The transformation $\hat{\mathcal{F}}$ (2.2) represents this very reparameterization group in the space of fields ϕ_i (*the scalar basis*) supplemented by $U(1)$ symmetry group with parameter ρ_0, which describes *an overall phase freedom*.

By construction, the Lagrangian of the form (2.1) with coefficients λ_i, m^2_{ij} and that with coefficients λ_i', $(m')^2_{ij}$ given by Eq. (2.3) describe the same physical reality. We call this property a *reparameterization invariance*.

A set of physically equivalent Higgs Lagrangians, obtained from each other by the transformations (2.3), forms *the reparameterization equivalent space*, being a three-dimensional subspace of the entire space of Lagrangians—Fig. 1. The parameters of Lagrangian can be determined from measurements in principle only with accuracy up to the reparameterization freedom; the different Lagrangians within the reparameterization equivalent space are physically equivalent.

All in principle observable quantities are invariants of reparameterization transformations (IRpaT), that are, for example, masses of observable Higgs bosons. Each of them is determined as eigenvalues of mass matrix (4.5) and (4.3). The coefficients of secular equations for diagonalization of this mass matrix (4.5) (among them—trace of this matrix and its determinant) can be constructed from these eigenvalues. Therefore, they are also IRpaT. The same is valid for the eigenvalues of Higgs-Higgs scattering matrices. The set of these IRpaT, classified in respect of isospin and hypercharge of Higgs-Higgs system, is presented in Ref. [7].

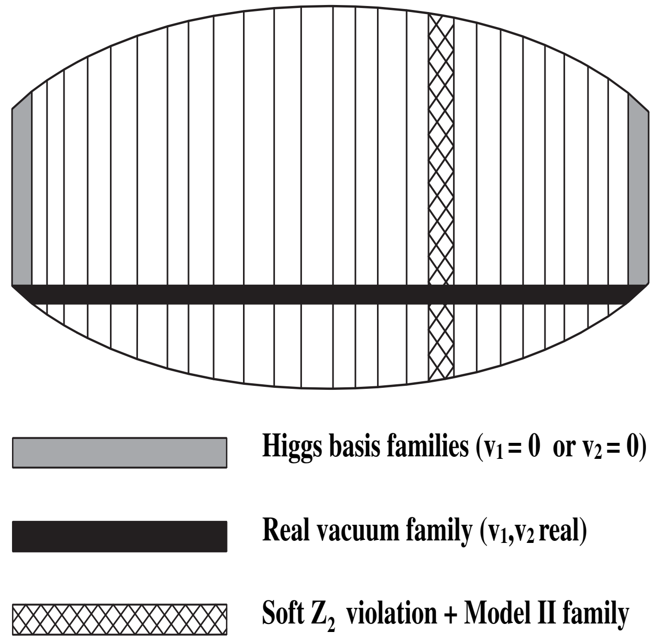

FIG. 1. Schematic presentation of reparameterization equivalent space of Lagrangians. Different strips represent families with different explicit properties. A particular case when the soft Z_2-violating and model II Lagrangians families coincide is shown.

The approach for construction of IRpaT is proposed in [8]. The group-theoretical approach for construction of all independent invariants of this transformation is presented in Ref. [9].

Remark on the $\varkappa \neq 0$ case.—The transformation (2.2) induces for $\varkappa \neq 0$ change of the kinetic term (2.1b):

$$\begin{aligned}
T = {}& z_1^{-1}(D_\mu\phi_1')^\dagger(D^\mu\phi_1') + z_2^{-1}(D_\mu\phi_2')^\dagger(D^\mu\phi_2')\\
&+ \varkappa'(D_\mu\phi_1')^\dagger(D^\mu\phi_2') + \varkappa'^*(D_\mu\phi_2')^\dagger(D^\mu\phi_1'),
\end{aligned} \tag{2.4}$$

with

$$z_1^{-1} = 1 - 2cs\,\mathrm{Re}(e^{-i\tau}), \qquad z_2^{-1} = 1 + 2cs\,\mathrm{Re}(e^{-i\tau}\varkappa),$$
$$\varkappa' = e^{-i\rho}(c^2\varkappa - s^2 e^{2i\tau}\varkappa^*).$$

So, in order to restore a canonical form of the kinetic term a field renormalization is needed in addition to the transformations (2.3). This case will be discussed in more detail elsewhere.

Remark on physical parameters.—Some parameters of theory which are treated often as physical (and in principle measurable) ones are in fact reparameterization dependent. The most important example provides a ratio of vacuum expectation values of scalar fields, $\tan\beta$ (3.7). For example, under the transformation (2.2) with $\rho = \xi$ [see Eq. (3.7b)] and $\tau = 0$, angle β changes to $\beta + \theta$.

2. Rephasing invariance

It is useful to consider a particular case of the transformations (2.2) with $\theta = 0$. It also can be treated as a global transformation of fields with independent phase rotations (*rephasing transformation of the fields*):

$$\phi_k \to e^{-i\rho_i}\phi_k, \qquad (k = 1, 2), \qquad \rho_1 = \rho_0 - \frac{\rho}{2}, \qquad \rho_2 = \rho_0 + \frac{\rho}{2}, \qquad \rho = \rho_2 - \rho_1. \tag{2.5}$$

This transformation leads to a change of phase of some coefficients of Lagrangian [*the rephasing transformation (RPhT) of the parameters*]:

$$\lambda_{1-4} \to \lambda_{1-4}, \qquad m_{11}^2 \to m_{11}^2, \qquad m_{22}^2 \to m_{22}^2, \qquad \lambda_5 \to \lambda_5 e^{-2i\rho}, \qquad \lambda_{6,7} \to \lambda_{6,7} e^{-i\rho}, \qquad m_{12}^2 \to m_{12}^2 e^{-i\rho}, \qquad \varkappa \to \varkappa e^{-i\rho}. \tag{2.6}$$

By construction, the Lagrangian of the form (2.1) with coefficients λ_i, m_{ij}^2 and that with coefficients given by Eq. (2.6) describe the same physical reality. We call this property a *rephasing invariance*; it is similar to the definition given in [10].

The transformations (2.6) represent the one-parametrical *rephasing transformation group* with parameter ρ. By construction, this group is a subgroup of the reparameterization transformation group.

The one-dimensional *rephasing equivalent space* is a subspace of the entire three-dimensional reparameterization equivalent space of Lagrangians. The rephasing equivalent space is given by the sets of parameters of Lagrangians at different ρ. One can say that the entire reparameterization equivalent space is sliced to the rephasing equivalent subspaces (represented by the vertical strips in Fig. 1).

Remarks.—The concept of the rephasing invariance is easily extended to the description of a whole system of scalars and fermions by adding to the transformation (2.6) transformations (5.2b) for the Yukawa parameters.

The transformation for scalar fields (2.2) evidently induces changes into the set of Yukawa parameters. This may hide some properties of the Yukawa Lagrangian, which are explicit in a definite scalar basis (e.g. model I or model II, see Sec. V). The Kobyashi-Maskawa matrix represents the reparameterization transformation from the quark basis of QCD to the electroweak basis.

We will see that *CP* symmetry is conserved in the Higgs sector if there exists a Lagrangian in the form (2.1) with all parameters real. Obviously, this violation does not appear if the Lagrangian with complex parameters can be transformed by means of some RPaT (2.3) to a form with all parameters real.

B. Lagrangian and Z_2 symmetry

The violation of the Z_2 symmetry (1.2) in the Lagrangian allows for the $\phi_1 \leftrightarrow \phi_2$ transitions. The general Higgs Lagrangian $\mathcal{L}_H$ (2.1) violates Z_2 symmetry by terms of the operator dimension 2 (with m_{12}^2), what is called *a soft violation of Z_2 symmetry*, and of the operator dimension 4 (with $\lambda_{6,7}$ and $\varkappa$), called *a hard violation of Z_2 symmetry.*

(a) *An exact* $\mathbf{Z}_2$ *symmetry.*—This case is described by the Lagrangian $\mathcal{L}_H$ (2.1) with $\lambda_6 = \lambda_7 = \varkappa = m_{12}^2 = 0$ and only one parameter λ_5 can be complex. The RPhT (2.6) with a suitable phase ρ allows to get another form of Lagrangian with a real λ_5, within the rephasing invariant space.

(b) *A soft violation of* $\mathbf{Z}_2$ *symmetry.*—In the case of soft violation of Z_2 symmetry one adds to the Z_2 symmetric Lagrangian the term $m_{12}^2(\phi_1^\dagger\phi_2) + \text{H.c.}$, with a generally complex m_{12}^2 (and λ_5) parameter. This type of violation respects the Z_2 symmetry at small distances (much smaller than $1/M$) in all orders of perturbative series, i.e. the amplitudes for $\phi_1 \leftrightarrow \phi_2$ transitions disappear at virtuality $k^2 \sim M^2 \to \infty$. That is the reason for the name—a "soft" violation. The RPhT's (2.6) applied to the Lagrangian with a softly violated Z_2 symmetry cannot change its character; they generate a whole *soft Z_2 violating Lagrangian family* (the crossed "vertical" strip in Fig. 1).

(c) *A hard violation of Z_2 symmetry.*—In the general case the terms of the operator dimension 4, with generally complex parameters λ_6, λ_7, and $\varkappa$, are added to the Lagrangian with a softly violated Z_2 symmetry. This is called a hard violation of Z_2 symmetry.
This case includes both the opportunity of a hidden soft Z_2 symmetry violation (obtained from an exact or softly violated Z_2 symmetry case by a general RPaT) and of *the true hard violation of Z_2 symmetry*, which cannot be transformed to the case of exact or softly violated Z_2 symmetry by any RPaT (2.3). In the latter case the Z_2 symmetry is broken *at both large and small distances* in any scalar basis.

1. The case of a hidden soft Z_2 violation

Let our physical system be described by the Lagrangian with exact or softly violated Z_2 symmetry $\mathcal{L}_s$. The general RPaT (2.3) converts this Lagrangian to a form $\mathcal{L}_{hs}$ with $\lambda_6, \lambda_7 \neq 0$ and $\varkappa = 0$. We call $\mathcal{L}_{hs}$ a Lagrangian with a *hidden soft Z_2 violation*.

To simplify discussion of such a case we first apply to $\mathcal{L}_s$ the RPhT (2.6) to eliminate the phase of λ_5. We obtain the Lagrangian $\mathcal{L}_s^R$ with real λ_5 (still m_{12}^2 can be complex leaving open an opportunity for *CP* violation). Then we apply to $\mathcal{L}_s^R$ a general RPaT (2.3) and obtain Lagrangian

$\mathcal{L}_{hs}$ in the form (2.1), with generally complex λ_5 and nonzero $\lambda_{6,7}$ (but still $\varkappa = 0$). We get from (2.3)

$$\begin{aligned}
&\lambda_1' = c^2\lambda_1 + s^2\lambda_2 - cs\Phi,\\
&\lambda_2' = s^2\lambda_1 + c^2\lambda_2 - cs\Phi, \qquad \lambda_3' = \lambda_3 + cs\Phi,\\
&\lambda_4' = \lambda_4 + cs\Phi,\\
&\lambda_5' = e^{-2i\rho}\lambda_5 + e^{2i\tau}[cs\Phi + 2is^2\lambda_5 \sin 2\tau],\\
&\lambda_6' = \frac{e^{i(\tau-\rho)}}{2}[cs(\lambda_1 - \lambda_2) + A],\\
&\lambda_7' = \frac{e^{i(\tau-\rho)}}{2}[cs(\lambda_1 - \lambda_2) - A],\\
&\quad \text{with } A = (c^2 - s^2)\Phi + 2ics\lambda_5 \sin 2\tau,\\
&\Phi = cs[\lambda_1 + \lambda_2 - 2(\lambda_3 + \lambda_4 + \lambda_5 \cos 2\tau)].
\end{aligned} \tag{2.7}$$

The Eqs. (2.7) allow to find parameters of the Lagrangian $\mathcal{L}_s^R$ with the explicit soft violating Z_2 symmetry and real λ_5, once the parameters of $\mathcal{L}_{hs}$ are known. The procedure is as follows:

(1) The value of $\tau - \rho$ is determined from the equation

$$\frac{\lambda_6' + \lambda_7'}{\lambda_6'^* + \lambda_7'^*} = e^{2i(\tau-\rho)}. \tag{2.8a}$$

(2) After that one can determine angle θ via equation

$$\frac{\lambda_6' + \lambda_7'}{\lambda_1' - \lambda_2'} = e^{i(\tau-\rho)}\frac{\tan 2\theta}{2}. \tag{2.8b}$$

(3) Next one can determine quantity Φ and $2cs\lambda_5 \sin 2\tau$ via the real and imaginary parts of

$$e^{-i(\tau-\rho)}(\lambda_6' - \lambda_7') = (c^2 - s^2)\Phi + 2ics\lambda_5 \sin 2\tau. \tag{2.8c}$$

(4) Then one can determine the angle ρ and the parameter λ_5 as the phase and the module of the quantity

$$e^{-i\rho}\lambda_5 = \lambda_5' - e^{2i(\tau-\rho)}[cs\Phi + 2is^2 \sin 2\tau\lambda_5]. \tag{2.8d}$$

(5) Finally, all remaining quantities λ_{1-4} can be determined easily from the first four Eqs. (2.7).

Equations (2.8c) and (2.8d) represent two different ways of obtaining the parameter λ_5. Besides, quantity Φ can be obtained both via Eq. (2.8c) and from the basic definition $\Phi = \lambda_1 + \lambda_2 - 2[\lambda_3 + \lambda_4 + \lambda_5 \cos 2\tau]$. The existence of these two ways can be considered as two constraints on the Lagrangian. It shows explicitly that in this case the quartic sector is described by only eight independent parameters (λ_{1-5} and θ, ρ, τ) instead of 10 independent parameters of the general Lagrangian (2.1) (λ_{1-4}, Reλ_{5-7}, Imλ_{5-7}).

2. Some features of the true hard Z_2 violation

The most general Higgs Lagrangian (2.1) cannot be transformed to the form with $\lambda_6 = \lambda_7 = 0$ by any RPaT. We denote this case as that with *true hard Z_2 symmetry violation*. Let us discuss briefly what should be done in this case with the mixed kinetic terms in Eq. (2.1b). First we observe that this mixed kinetic term can be removed by the nonunitary transformation, e.g.

$$(\phi_1', \phi_2') \to \left(\frac{\sqrt{\varkappa^*}\phi_1 + \sqrt{\varkappa}\phi_2}{2\sqrt{|\varkappa|(1+|\varkappa|)}} \pm \frac{\sqrt{\varkappa^*}\phi_1 - \sqrt{\varkappa}\phi_2}{2\sqrt{|\varkappa|(1-|\varkappa|)}}\right). \tag{2.9}$$

However, in presence of the λ_6 and λ_7 terms, the renormalization of quadratically divergent, nondiagonal two-point functions leads anyway to the mixed kinetic terms (e.g. from loops with $\lambda_6^*\lambda_{1,3-5}$ and $\lambda_7^*\lambda_{2-5}$). It means that $\varkappa$ becomes nonzero at the higher orders of perturbative theory, and *vice versa* a mixed kinetic term generates counterterms with $\lambda_{6,7}$. Therefore all of these terms should be included in Lagrangian (2.1a) on the same footing, i.e. the treatment of the hard violation of Z_2 symmetry without $\varkappa$ terms is inconsistent (see also [11,12]). (The phenomenon is analogous to a need of a quartic coupling of the form $\lambda\phi^4$ in the renormalization of the $\bar\psi\gamma^5\psi\phi$ theory [13].) Note that the parameter $\varkappa$ is generally running like parameters λ's. Therefore, the Lagrangian *remains off diagonal* in fields $\phi_{1,2}$ even at very small distances, above the EWSB transition. Such theory seems to be *unnatural*.

When finding a signature of this case in the arbitrary form of Lagrangian it is useful to consider a polarization operator matrix for two fields:

$$\mathcal{P} = \begin{pmatrix} \Pi_{11} & \Pi_{12} \\ \Pi_{21} & \Pi_{22} \end{pmatrix}.$$

In the general case the ratio $\Pi_{12}/(\Pi_{11} - \Pi_{22})$ is a running quantity at large Higgs boson virtuality k^2 in contrast to the case of a hidden Z_2 symmetry, where this ratio is not running.

Indeed, let us consider the Lagrangian with soft violation of Z_2 symmetry, $\mathcal{L}_s$, like in Sec. III. The one-loop polarization operator matrix for two fields has a form

$$\mathcal{P} = \begin{pmatrix} \Pi_1^s & 0 \\ 0 & \Pi_2^s \end{pmatrix} k^2 + \text{ finite terms},$$

for $k^2 \to \infty$. The elements Π_1^s and Π_2^s describe renormalization of fields ϕ_1 and ϕ_2, respectively. There is no mixed kinetic term, and the $\phi_1 \leftrightarrow \phi_2$ transitions at small distances are absent.

Under RPaT, the $\mathcal{L}_s$ is converted to the Lagrangian $\mathcal{L}_{hs}$, with nonzero λ_6 and λ_7 terms (2.7), still with $\varkappa = 0$. This Lagrangian leads to the polarization operator with a nonzero mixed term:

$$\mathcal{P}'k^2 = \begin{pmatrix} \Pi_1^s\cos^2\theta + \Pi_2^s\sin^2\theta & \Pi_{12} \\ \Pi_{12}^* & \Pi_2^s\cos^2\theta + \Pi_1^s\sin^2\theta \end{pmatrix}$$

with $\Pi_{12} = (\Pi_1^s - \Pi_2^s)e^{-i\tau}\sin\theta\cos\theta$. Naïvely, this form of the polarization operator suggests that one should introduce in the Lagrangian the mixed kinetic term describing transitions $\phi_1' \leftrightarrow \phi_2'$. However, the renormalization group analysis ensures that in this case the ratio $\Pi_{12}/(\Pi_{11} - \Pi_{22})$ at large k^2 is renormalization invariant quantity (in contrast to the mentioned above case of the true hard violation of Z_2 symmetry). In such case there exist some parameters ρ, θ, τ which restore the incident form of $\mathcal{L}_H$ with soft Z_2 symmetry violation, i.e. without kinetic terms. In such scalar basis the transitions $\phi_1 \leftrightarrow \phi_2$ are absent at small distances. Since the kinetic term of Lagrangian can be obtained from the initial diag(1, 1) form by the orthogonal transformation (2.2), one can conclude that the mentioned relations among parameters of new quartic terms prevent an appearance of the mixed kinetic term in the Higgs Lagrangian in any reparameterization equivalent Lagrangians. As it was mentioned above, this is in contrast to the general case with the true hard violation of Z_2 symmetry, where $\phi_1 \leftrightarrow \phi_2$ transitions at different large k^2 cannot be ruled out simultaneously by any RPaT (2.3).

The other example is given by the EWSB procedure (Sec. III) in the case of soft violation of Z_2 symmetry. It transforms the Lagrangian expressed in terms of fields $\phi_{1,2}$ to that written in terms of Higgs fields h_{1-3} and $H^\pm$. In this form many quartic couplings appear but there are some relations among them, since all of them were obtained from the initial Lagrangian $\mathcal{L}_s$ with six parameters (λ_{1-4}, Reλ_5, Imλ_5) and the orthogonal transformation from the (ϕ_1, ϕ_2) basis to $(H^\pm, h_1, h_2, h_3)$ basis with the additional three parameters. In this Lagrangian a mixed polarization operator may appear also but no mixed kinetic term in contrast to the case of true hard violation of Z_2 symmetry. This is due to the mentioned relations among parameters of new quartic terms which prevent appearance of the mixed kinetic term in the Higgs Lagrangian [14]. The detailed discussion of these problems will be done elsewhere.

Other aspects of the hard violation of Z_2 symmetry are related to the description of Yukawa sector. This will be discussed in Sec. V.

Remarks.—The diagonalization described by Eq. (2.9) is rather special and it changes even the definitions of λ's, that would destroy relatively simple relations between the masses of the Higgs bosons discussed below.

Although in this paper we present relations for the case of hard violation of Z_2 symmetry at $\varkappa = 0$ one should keep in mind that loop corrections can change results significantly. *Such treatment of the case with hard violation of Z_2 symmetry is as incomplete as in most of the papers considering this "most general 2HDM potential."* A full treatment of this problem goes beyond the scope of the present paper.

III. VACUUM

The extremes of the potential define the vacuum expectation values (v.e.v.'s $\langle\phi_{1,2}\rangle$) of the fields $\phi_{1,2}$ via equations:

$$\frac{\partial V}{\partial \phi_1}\bigg|_{\substack{\phi_1=\langle\phi_1\rangle,\\ \phi_2=\langle\phi_2\rangle}} = 0, \qquad \frac{\partial V}{\partial \phi_2}\bigg|_{\substack{\phi_1=\langle\phi_1\rangle,\\ \phi_2=\langle\phi_2\rangle}} = 0. \tag{3.1}$$

This equation has trivial electroweak symmetry conserving solution $\langle\phi_1\rangle = 0$, $\langle\phi_2\rangle = 0$ and electroweak symmetry violating solutions, discussed below. With accuracy to the choice of z axis in the weak isospin space, and using the overall phase freedom of the Lagrangian to choose one vacuum expectation value real, most general electroweak symmetry violating solution can be written in a form

$$\langle\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_1 \end{pmatrix}, \qquad \langle\phi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} u \\ v_2 e^{i\xi} \end{pmatrix}. \tag{3.2}$$

It is useful to describe the discussed extremes with the aid of quantities

$$\begin{aligned} y_1 &= \langle\phi_1^\dagger\rangle\langle\phi_1\rangle, \qquad y_2 = \langle\phi_2^\dagger\rangle\langle\phi_2\rangle, \\ y_3 &= \langle\phi_1^\dagger\rangle\langle\phi_2\rangle, \qquad y_3 y_3^* - y_1 y_2. \end{aligned} \tag{3.3}$$

A. $u \neq 0$ solution, charged vacuum

For

$$y_3^* y_3 - y_1 y_2 \neq 0 \quad \text{we have } u \neq 0. \tag{3.4}$$

In this case the v.e.v.'s are given by equations

$$\begin{aligned} &\lambda_1 y_1 + \lambda_3 y_2 + \lambda_6^* y_3^* + \lambda_6 y_3 = m_{11}^2/2, \\ &\lambda_2 y_2 + \lambda_3 y_1 + \lambda_7^* y_3^* + \lambda_7 y_3 = m_{22}^2/2, \\ &\lambda_4 y_3^* + \lambda_5 y_3 + \lambda_6 y_1 + \lambda_7 y_2 = m_{12}^2/2. \end{aligned} \tag{3.5}$$

Depending on the parameters of potential, the extremum given by this solution of (3.1) describes either saddle point or a minimum of the potential, denoted as *a charged vacuum*, with a heavy photon and other nonphysical properties [15,16].

B. $u = 0$ solution, physical (neutral) vacuum

Another solution of extremum condition (3.1) is realized at

$$y_3^* y_3 - y_1 y_2 = 0, \quad \text{which gives } u = 0. \tag{3.6}$$

The solution has a form

$$\langle\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_1 \end{pmatrix} \quad \text{and} \quad \langle\phi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v_2 e^{i\xi} \end{pmatrix}. \tag{3.7a}$$

It satisfies a condition for $U(1)$ symmetry of electromagnetism. This extremum realizes minimum of potential if its parameters are such that all eigenvalues of mass-squared matrix in this extremum point are nonnegative, as in Sec. VI B. In the analysis we consider only this very case. (At this set of parameters the vacuum energy corresponding to the solution (3.5) is larger than that for the solution (3.7) [15,16].) The v.e.v's $v_{1,2}$ (and therefore parameters of whole Lagrangian) obey the SM constraint: $v_1^2 + v_2^2 = v^2$, with $v = (\sqrt{2}G_F)^{-1/2} = 246$ GeV. The other parameterization of these v.e.v.'s is also used:

$$v_1 = v\cos\beta, \qquad v_2 = v\sin\beta, \qquad \beta \in \left(0, \frac{\pi}{2}\right). \tag{3.7b}$$

The rephasing of fields (2.5) shifts the phase difference ξ as

$$\xi \to \xi - \rho. \tag{3.8}$$

Therefore, the phase difference ξ between the v.e.v.'s has no physical sense (it was discussed e.g. in [10]).

The arbitrariness described by (3.8) allows to simplify further calculations in a following way. Let us take some Lagrangian describing our model and calculate v.e.v.'s (3.7). Then, by making the RPhT with $\rho = \xi$, we get *the Lagrangian in a real vacuum form (a real vacuum Lagrangian)* (and *the potential in a real vacuum form*). By definition, the relative phase of v.e.v.'s derived from this Lagrangian equals zero. In accordance with Eq. (2.6) we get now

$$\begin{aligned} &\lambda_{1-4,rv} = \lambda_{1-4}, \qquad \lambda_{5,rv} = \lambda_5 e^{-2i\xi},\\ &\lambda_{6,rv} = \lambda_6 e^{-i\xi}, \qquad \lambda_{7,rv} = \lambda_7 e^{-i\xi},\\ &\varkappa_{rv} = \varkappa e^{-i\xi}, \qquad m_{12,rv}^2 = m_{12}^2 e^{-i\xi}, \end{aligned} \tag{3.9}$$

where we denote the particular values of parameters of such Lagrangian (potential) by subscript *rv*.

The following combinations of parameters and new quantities are useful:

$$\begin{aligned} &\lambda_{3,rv} + \lambda_{4,rv} + \mathrm{Re}\lambda_{5,rv} = \lambda_{345,rv},\\ &\frac{v_1}{v_2}\lambda_{6,rv} \pm \frac{v_2}{v_1}\lambda_{7,rv} = \begin{cases} \lambda_{67,rv},\\ \tilde{\lambda}_{67,rv}, \end{cases}\\ &m_{12,rv}^2 = 2v_1 v_2(\nu + i\delta). \end{aligned} \tag{3.10}$$

For given $v_{1,2}$ the extremum condition (3.1) does not constrain $\mathrm{Re}m_{12,rv}^2$, while it does so for $\mathrm{Im}m_{12,rv}^2$, allowing to express it via $\mathrm{Im}(\lambda_{5-7,rv})$:

$$\delta = \underbrace{0}_{Z_2\mathrm{sym}} + \underbrace{\tfrac{1}{2}\,\mathrm{Im}\lambda_{5,rv}}_{\mathrm{soft}} + \underbrace{\tfrac{1}{2}\,\mathrm{Im}\lambda_{67,rv}}_{\mathrm{hard}}. \tag{3.11}$$

Here (and in the subsequent equations) the first underbraced term corresponds to the Z_2 symmetric case, the second and third terms are added to each other in the case of explicitly soft and hard violations of Z_2 symmetry, respectively. In particular, in the Z_2 symmetric case $m_{12,rv}^2 = 0$ and consequently $\mathrm{Im}\lambda_{5,rv} = 0$.

Beginning from here all expressions will be presented for the potential in a real vacuum form, without writing explicitly the subscript rv. We will explicitly comment when other forms of Lagrangian will be discussed.

Remarks.—The set of real vacuum Lagrangians forms a subspace in the entire reparameterization equivalent space—*the real vacuum Lagrangian family.* It is pictured in Fig. 1 by the black horizontal line. In different points of this subspace the $\tan\beta$ values are different.

C. Our form of the potential

It is useful for the subsequent calculations to describe the potential in terms of v_1, v_2, and ν instead of three quadratic parameters $m_{11,22}^2$, m_{12}^2 [17]. The Eqs. (3.1) and (3.10) allow us to obtain relations

$$\begin{aligned} m_{11}^2 &= \underbrace{\lambda_1 v_1^2 + \lambda_{345} v_2^2}_{Z_2\mathrm{sym}} - \underbrace{2\nu v_2^2}_{\mathrm{soft}} + \underbrace{\frac{v_2}{v_1}\mathrm{Re}(3v_1^2\lambda_6 + v_2^2\lambda_7)}_{\mathrm{hard}},\\ m_{22}^2 &= \underbrace{\lambda_2 v_2^2 + \lambda_{345} v_1^2}_{Z_2\mathrm{sym}} - \underbrace{2\nu v_1^2}_{\mathrm{soft}} + \underbrace{\frac{v_1}{v_2}\mathrm{Re}(v_1^2\lambda_6 + 3v_2^2\lambda_7)}_{\mathrm{hard}}. \end{aligned} \tag{3.12}$$

From these relations we obtain another form of real vacuum potential, used in this paper:

$$\begin{aligned} V = {}& \frac{\lambda_1}{2}\left[(\phi_1^\dagger\phi_1) - \frac{v_1^2}{2}\right]^2 + \frac{\lambda_2}{2}\left[(\phi_2^\dagger\phi_2) - \frac{v_2^2}{2}\right]^2 + \lambda_3(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_4(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) + \frac{1}{2}[\lambda_5(\phi_1^\dagger\phi_2)^2 + \mathrm{H.c.}]\\ &+ \{[\lambda_6(\phi_1^\dagger\phi_1) + \lambda_7(\phi_2^\dagger\phi_2)](\phi_1^\dagger\phi_2) + \mathrm{H.c.}\} - \frac{1}{2}(\lambda_{345} + 2\,\mathrm{Re}\lambda_{67})[v_2^2(\phi_1^\dagger\phi_1) + v_1^2(\phi_2^\dagger\phi_2)]\\ &- \mathrm{Re}[\lambda_6(\phi_1^\dagger\phi_1) + \lambda_7(\phi_2^\dagger\phi_2)]v_1v_2 + \nu(v_2\phi_1 - v_1\phi_2)^\dagger(v_2\phi_1 - v_1\phi_2) + 2\delta\,\mathrm{Im}(\phi_1^\dagger\phi_2)v_1v_2 - \lambda_1\frac{v_1^4}{8} - \lambda_2\frac{v_2^4}{8}. \end{aligned} \tag{3.13}$$

In this form the quartic terms are as those in the initial potential (2.1) but with particular values of parameters λ_i equal to $\lambda_{i,rv}$ (3.9). The mass term is determined via v.e.v.'s v_1, v_2 and the parameters λ_i plus a *single free* dimensionless parameter ν. The quantity $\delta \propto \mathrm{Im} m_{12}^2$ is given by Eq. (3.11). (Sometimes instead of ν a dimensional parameter μ, defined via $\mu^2 = \nu v^2$, is used.)

In the above equation the soft Z_2-violating contribution is written as a sum of two terms, so that the variation of each of them do not influence v.e.v.'s. The derivatives of first term ($\propto \nu$) over ϕ_k are equal to zero at the extremum point $\langle\phi_k\rangle = v_k/\sqrt{2}$. The second term ($\propto \delta$) is equal to zero for real $\phi_{1,2}$, independently on their absolute values. This decomposition is less transparent in Lagrangians with $\xi \neq 0$.

The vacuum energy density given by minimum (3.7) is equal to

$$\begin{aligned} E_{\mathrm{vac}} &\equiv V(\langle\phi_1\rangle, \langle\phi_2\rangle) \\ &= -\frac{\lambda_1 v_1^4}{8} - \frac{\lambda_2 v_2^4}{8} - \lambda_{345}\frac{v_1^2 v_2^2}{4} \\ &\quad - \Re(\lambda_6 v_1^2 + \lambda_7 v_2^2)\frac{v_1 v_2}{2}. \end{aligned} \tag{3.14}$$

Remark.—The transformation (2.2) with $\tau = 0$, $\theta = -\beta$, or $\theta = \pi/2 - \beta$ gives ($v_1 = v$, $v_2 = 0$) or ($v_1 = 0$, $v_2 = v$), respectively. The sets of the obtained Lagrangians form *Higgs basis Lagrangian families*; they are pictured as gray shaded vertical strips in the reparameterization equivalent Lagrangian space presented in Fig. 1. These cases cannot be described by our potential (3.13) since some of the coefficients (3.10) and (3.11), used at the transformation to this form, are singular at $v_2 \to 0$ or $v_1 \to 0$. For both of these cases $\sin 2\beta = 0$. Therefore, our analysis based on the potential (3.13) is valid only for Lagrangians with

$$\sin 2\beta \neq 0 \tag{3.15}$$

(domain of entire reparameterization equivalent space of Fig. 1 between two gray strips). Some results for the Higgs basis Lagrangian can be found in [10,18,19].

IV. PHYSICAL HIGGS SECTOR

The fields $\phi_{1,2}$ change under the transformation (2.2). We introduce now the, in principle, observable Higgs fields and their couplings. These fields and couplings are evidently reparameterization independent. (The reparameterization dependent are parameters describing the transformation to this physical basis, see below.)

A standard decomposition of the fields $\phi_{1,2}$ in terms of component fields is made via

$$\phi_1 = \begin{pmatrix} \varphi_1^+ \\ \dfrac{v_1 + \eta_1 + i\chi_1}{\sqrt{2}} \end{pmatrix}, \qquad \phi_2 = \begin{pmatrix} \varphi_2^+ \\ \dfrac{v_2 + \eta_2 + i\chi_2}{\sqrt{2}} \end{pmatrix}. \tag{4.1}$$

At $\varkappa = 0$ such decomposition leads to a diagonal form of kinetic terms for new fields φ_i^+, χ_i, η_i, while the corresponding mass matrix is off diagonal. The mass-squared matrix can be transformed to the block diagonal form by a separation of the massless Goldstone boson fields, $G^0 = \cos\beta\chi_1 + \sin\beta\chi_2$ and $G^\pm = \cos\beta\varphi_1^\pm + \sin\beta\varphi_2^\pm$, and the charged Higgs boson fields $H^\pm$:

$$H^\pm = -\sin\beta\varphi_1^\pm + \cos\beta\varphi_2^\pm, \tag{4.2}$$

with the mass-squared equal to

$$M_{H^\pm}^2 = \left[\nu - \tfrac{1}{2}(\lambda_4 + \mathrm{Re}\lambda_5 + \mathrm{Re}\lambda_{67})\right]v^2. \tag{4.3}$$

A. Neutral Higgs sector—general introduction

By definition $\eta_{1,2}$ are the standard C- and P-even (scalar) fields. The field

$$A = -\sin\beta\chi_1 + \cos\beta\chi_2, \tag{4.4}$$

is C-odd (which in the interactions with fermions behaves as a P-odd particle, i.e. a pseudoscalar). In other words, the $\eta_{1,2}$ and A are fields with opposite CP parities (see e.g. [1] for details). (Note that sometimes the set η_1, η_2, and A is called the weak basis [10].)

The decomposition (4.1) results in the (symmetric) mass-squared matrix $\mathcal{M}$ in the η_1, η_2, A basis

$$\mathcal{M} = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{12} & M_{22} & M_{23} \\ M_{13} & M_{23} & M_{33} \end{pmatrix}, \tag{4.5a}$$

with

$$\begin{aligned} M_{11} &= \left[c_\beta^2\lambda_1 + s_\beta^2\nu + s_\beta^2\,\mathrm{Re}\left(\frac{\lambda_{67}}{2} + \tilde{\lambda}_{67}\right)\right]v^2, \\ M_{22} &= \left[s_\beta^2\lambda_2 + c_\beta^2\nu + c_\beta^2\,\mathrm{Re}\left(\frac{\lambda_{67}}{2} - \tilde{\lambda}_{67}\right)\right]v^2, \\ M_{33} &= \left[\nu - \mathrm{Re}\left(\lambda_5 - \frac{1}{2}\lambda_{67}\right)\right]v^2, \\ M_{12} &= -\left[\nu - \lambda_{345} - \frac{3}{2}\,\mathrm{Re}\lambda_{67}\right]c_\beta s_\beta v^2, \\ M_{13} &= -\left[\delta + \frac{1}{2}\,\mathrm{Im}\tilde{\lambda}_{67}\right]s_\beta v^2, \\ M_{23} &= -\left[\delta - \frac{1}{2}\,\mathrm{Im}\tilde{\lambda}_{67}\right]c_\beta v^2, \end{aligned} \tag{4.5b}$$

where we use abbreviations $c_\beta = \cos\beta$, $s_\beta = \sin\beta$. As we discuss below M_{33} is equal to the mass-squared of the CP-odd Higgs boson in the CP-conserving case, namely,

$$M_A^2 = M_{33} = [\nu - \mathrm{Re}(\lambda_5 - \tfrac{1}{2}\lambda_{67})]v^2. \tag{4.5c}$$

The masses squared M_i^2 of the physical neutral states h_{1-3} are eigenvalues of the matrix $\mathcal{M}$. These states are obtained from fields η_1, η_2, A by a unitary transformation R which diagonalizes the matrix $\mathcal{M}$:

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R \begin{pmatrix} \eta_1 \\ \eta_2 \\ A \end{pmatrix}, \quad \text{with } R\mathcal{M}R^T = \mathrm{diag}(M_1^2, M_2^2, M_3^2). \tag{4.6}$$

The diagonalizing matrix R can be written as a product of three rotation matrices described by three Euler angles $\alpha_i \in (0, \pi)$ (we define $c_i = \cos\alpha_i$, $s_i = \sin\alpha_i$):

$$R = R_3R_2R_1, \qquad R_1 = \begin{pmatrix} c_1 & s_1 & 0 \\ -s_1 & c_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad R_2 = \begin{pmatrix} c_2 & 0 & s_2 \\ 0 & 1 & 0 \\ -s_2 & 0 & c_2 \end{pmatrix}, \qquad R_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_3 & s_3 \\ 0 & -s_3 & c_3 \end{pmatrix}, \tag{4.7a}$$

$$R = \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \equiv \begin{pmatrix} c_1c_2 & c_2s_1 & s_2 \\ -c_1s_2s_3 - c_3s_1 & c_1c_3 - s_1s_2s_3 & c_2s_3 \\ -c_1c_3s_2 + s_1s_3 & -c_1s_3 - c_3s_1s_2 & c_2c_3 \end{pmatrix}. \tag{4.7b}$$

We adopt the convention for masses that $M_2 \geq M_1$ but shall *not* require any other ordering.

Remarks.—Note that in the case where there is an exact Z_2 symmetry and $\lambda_5 = 0$ there appears an additional Peccei-Quinn symmetry. Then A is a massless Goldstone-like boson, $M_A = 0$. The spontaneous violation of this symmetry results in a light particle with mass, which is generated due to nonperturbative effects.

For the basic Higgs Lagrangian (2.1) in the case of a soft violation of Z_2 symmetry and model II or I for the Yukawa interaction (see below), the perturbative corrections give no counterterms violating the Z_2 symmetry in a hard way. Therefore, with a suitable renormalization procedure, the mixed kinetic terms do not appear in the Lagrangian in h_{1-3} basis [the rotation (4.6) keeps kinetic term diagonal in all orders]. At the same time, the mass terms and mixing angles α_i change due to the renormalization. Some aspects of this procedure were discussed in [14].

B. Condition for *CP* violation

In general, the obtained Higgs eigenstates h_i (4.6) have no definite CP parity since they are mixtures of fields $\eta_{1,2}$ and A having the opposite CP parities. This provides a CP nonconservation within the Higgs sector.

The interaction of these Higgs bosons with matter explicitly violates the CP symmetry. Such mixing (and violation of CP) is absent if and only if $M_{13} = M_{23} = 0$. If $\sin2\beta \neq 0$ it means that $\mathrm{Im}\tilde{\lambda}_{67} = 0$ and $\delta \propto \mathrm{Im}(m_{12}^2) = 0$. From the (3.11) it follows that the CP violation is absent if all coefficients in potential of a real vacuum form are real. A simple but cumbersome calculation shows that a similar conclusion is valid also for the potential in a Higgs basis form, i.e. for $\sin2\beta = 0$. In other words, CP symmetry in the Higgs sector is not violated if among different reparameterization equivalent potentials a potential with all real λ_i, m_{ij}^2 parameters can be found.

Vice versa, the complexity of some parameters of the potential in *a real vacuum form* is a sufficient condition for CP violation in the Higgs sector. For an arbitrary form of Lagrangian (in entire reparameterization space) the necessary and sufficient condition for CP violation in the Higgs sector can be written as complexity of some of the combinations [which are invariant under RPhT; see (2.6)]

$$\lambda_5^*(m_{12}^2)^2, \qquad \lambda_6^*m_{12}^2, \qquad \lambda_7^*m_{12}^2. \tag{4.8}$$

The quantity of each is not a reparameterization invariant one but these forms are very simple. (For the soft Z_2 violated potential one should be $\mathrm{Im}\lambda_5^*(m_{12}^2)^2 \neq 0$—cf. [20].) The RPa invariant conditions for CP violation [2,8] are more complex.

C. Diagonalization of the scalar *CP*-even sector

It is useful to start with the diagonalization of scalar $\langle 12\rangle$ sector of matrix $\mathcal{M}$ which is given by the rotation matrix R_1. It results in the neutral, CP-even Higgs fields which we denote as h and $(-H)$, while the CP-odd field A remains unmixed. (Sign minus at H is needed in order to match a standard convention used for CP-conserving case, see e.g. [1].) We got

$$\begin{pmatrix} h \\ -H \\ A \end{pmatrix} = R_1 \begin{pmatrix} \eta_1 \\ \eta_2 \\ A \end{pmatrix}$$

$$\text{with } \mathrm{R}_1\mathcal{M}\mathrm{R}_1^{\mathrm{T}} = \mathcal{M}_1 \equiv \begin{pmatrix} \mathrm{M}_\mathrm{h}^2 & 0 & \mathrm{M}'_{13} \\ 0 & \mathrm{M}_\mathrm{H}^2 & \mathrm{M}'_{23} \\ \mathrm{M}'_{13} & \mathrm{M}'_{23} & \mathrm{M}_\mathrm{A}^2 \end{pmatrix}, \tag{4.9}$$

with M'_{13}, M'_{23} given in Eq. (4.14).

Let us stress that in the general CP nonconserving case the states h, H, and A have no direct physical sense, they are only subsidiary concepts useful in the calculations and *discussions.* In the case of CP conservation (realized for $M'_{13} = M'_{23} = 0$) the fields h, H, and A represent physical Higgs bosons: $h_1 = h$, $h_2 = -H$, $h_3 = A$. This is why we use instead of α_1 the mixing angle $\alpha \in (-\pi/2, \pi/2)$,

$$\alpha = \alpha_1 - \pi/2, \tag{4.10}$$

which is customary for the CP-conserving case. Using this angle we get

$$H = \cos\alpha\,\eta_1 + \sin\alpha\,\eta_2, \qquad h = -\sin\alpha\,\eta_1 + \cos\alpha\,\eta_2. \tag{4.11}$$

The diagonalization of the respective $\langle 12\rangle$ corner of mass-squared matrix $\mathcal{M}$ (4.5) results in

$$M^2_{h,H} = \tfrac{1}{2}(M_{11} + M_{22} \mp \mathcal{N}), \qquad \mathcal{N} = \sqrt{(M_{11} - M_{22})^2 + 4M^2_{12}}. \tag{4.12}$$

The following expressions for angles are useful in some applications:

$$\cos 2\alpha = \frac{M_{11} - M_{22}}{M_H^2 - M_h^2}, \qquad \sin 2\alpha = \frac{2M_{12}}{M_H^2 - M_h^2}, \qquad \frac{\sin 2\alpha}{\sin 2\beta} = \frac{(\lambda_{345} - \nu + 3/2\,\mathrm{Re}\lambda_{67})v^2}{M_H^2 - M_h^2}. \tag{4.13}$$

D. Complete diagonalization

The above diagonalization keeps, in general, two off-diagonal elements in matrix $\mathcal{M}_1$ (4.9):

$$\begin{aligned} M'_{13} &= c_1 M_{13} + s_1 M_{23} \\ &= -\left[\delta\cos(\beta+\alpha) - \frac{\mathrm{Im}\tilde\lambda_{67}}{2}\cos(\beta-\alpha)\right]v^2, \\ M'_{23} &= -s_1 M_{13} + c_1 M_{23} \\ &= \left[\delta\sin(\beta+\alpha) + \frac{\mathrm{Im}\tilde\lambda_{67}}{2}\sin(\beta-\alpha)\right]v^2. \end{aligned} \tag{4.14}$$

If at least one of these off-diagonal terms differs from zero, the additional diagonalization is necessary, and the mass eigenstates, being admixtures of CP-even and CP-odd states, violate the CP symmetry. In this case we express the physical Higgs boson states h_{1-3} via h, H, A:

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R_3 R_2 \begin{pmatrix} h \\ -H \\ A \end{pmatrix}$$

$$\text{with } R\mathcal{M}R^T = R_3 R_2 \mathcal{M}_1 R_2^T R_3^T = \begin{pmatrix} M_1^2 & 0 & 0 \\ 0 & M_2^2 & 0 \\ 0 & 0 & M_3^2 \end{pmatrix}. \tag{4.15}$$

The squared masses M_i^2 in Eq. (4.15) are the eigenvalues of the mass-squared matrix $\mathcal{M}$ (4.5), i.e. they are roots of the corresponding cubic equation (see the solution, e.g., in Ref. [21]). Note, that the trace of mass-squared matrix does not change under the unitary transformations. Therefore, we have *mass sum rule*

$$M_1^2 + M_2^2 + M_3^2 = M_h^2 + M_H^2 + M_A^2 = M_{11} + M_{22} + M_{33}. \tag{4.16}$$

The relation (4.15) allows us to discuss the general CP-violating case in terms customary for the CP-conserving one, i.e. with *parameters* M_H, M_h, M_A, and α. The angles α_2, α_3 describe mixing of the CP-even states (h, H) with the CP-odd state A.

E. Various cases of *CP* violation

Here we present various cases of CP violation.

If $\delta = 0$ *and* $\mathrm{Im}\tilde\lambda_{67} = 0$, CP symmetry is not violated. The h, H, and A are physical Higgs bosons, with masses given by Eqs. (4.12) and (4.5c), and $\alpha_2 = \alpha_3 = 0$.

If $\varepsilon_{13} = |M'_{13}/(M_A^2 - M_h^2)| \ll 1$ the Higgs boson h_1 practically coincides with h ($\alpha_2 \approx 0$). The interaction of h_1 with other particles respects CP-symmetry (with an accuracy $\sim\varepsilon_{13}$). The diagonalization of the residual $\langle 23\rangle$ corner of mass-squared matrix (4.9) with the aid of rotation matrix R_3 (4.7a) gives states h_2 and h_3. They are superpositions of H and A states with potentially large mixing angle α_3:

$$\tan 2\alpha_3 \approx \frac{-2M'_{23}}{M_A^2 - M_H^2}, \qquad \alpha_2 \approx 0. \tag{4.17a}$$

If $M_A \approx M_H$, the CP-violating mixing can be strong even at small but nonzero $|M'_{23}|/v^2$. The states h_2 and h_3 have no definite CP parity and the mass difference $|M_2^2 - M_3^2|$ is larger than $|M_H^2 - M_A^2|$.[3] For example, at $M_H \approx 300$ GeV, $|M_H - M_A| \approx 5$ GeV, and $M'_{23} \approx 0.02v^2$ we have $|M_2^2 - M_3^3| \approx 25$ GeV, $\sin 2\alpha_3 \approx 0.8$.

At the growth of $M_H \approx M_A$ the proper widths of H and A become large so that the H and A peaks overlap strongly. In such cases the tree approximation may be too rough for a reliable calculation of masses M_i and mixing angles. Therefore one should supplement the mass-squared matrix (4.5) by a (complex) matrix of Higgs polarization operators as is customary in the description of low energy phenomena (see discussion in Sec. VII A).

If $\varepsilon_{23} = |M'_{23}/(M_A^2 - M_h^2)| \ll 1$, the Higgs boson h_2 practically coincides with $-H$ ($\alpha_3 \approx 0$). The interaction of matter with h_2 does not violate CP symmetry. Similarly to the previous case, the diagonalization of the $\langle 13\rangle$ part of mass-squared matrix (4.9), with the aid of rotation matrix R_2(4.7a), gives states h_1 and h_3. They are superpositions of

[3]In this case one can hope to separate h_2 and h_3 at the muon collider (see [22] for the case without mixing) and to measure mixing angle α_3 via measuring of difference in effects of CP violation in the corresponding two peaks.

h and A states with potentially large mixing angle α_2:

$$\tan 2\alpha_2 \approx \frac{-2M'_{13}}{M_A^2 - M_h^2}, \qquad \alpha_3 \approx 0. \qquad (4.17b)$$

Similarly to the previous case, if $M_A \approx M_h$, the CP-violating mixing can be strong even at small M'_{13}/v^2.

The case of a weak CP violation combines both of the described above cases (4.17). If both $|M'_{13}| \ll |M_A^2 - M_h^2|$ and $|M'_{23}| \ll |M_A^2 - M_H^2|$ the CP-even states h, H are weakly mixed with the CP-odd state A, and parameters α_2 and α_3 are simultaneously small:

$$\begin{aligned} \tan\alpha_2 &\approx s_2 \approx \frac{-M'_{13}}{M_A^2 - M_h^2} \approx \alpha_2, \\ \tan\alpha_3 &\approx s_3 \approx \frac{-M'_{23}}{M_A^2 - M_H^2} \approx \alpha_3, \\ &(|\alpha_2|, |\alpha_3| \ll 1). \end{aligned} \qquad (4.18a)$$

To the second order in s_2 and s_3 the corresponding masses are

$$\begin{aligned} M_1^2 &= M_h^2 - s_2^2(M_A^2 - M_h^2), \\ M_2^2 &= M_H^2 - s_3^2(M_A^2 - M_H^2), \end{aligned} \qquad (4.18b)$$

with M_3 given by the sum rule (4.16) . In the particular case of *a soft violation of* Z_2 *symmetry* we have

$$s_2 \approx \delta\frac{\cos(\beta+\alpha)}{M_A^2 - M_h^2}v^2, \qquad s_3 \approx -\delta\frac{\sin(\beta+\alpha)}{M_A^2 - M_H^2}v^2. \qquad (4.18c)$$

The case of *intense coupling regime* with $M_A \approx M_h \approx M_H$ [23] may also give strong CP-violating mixing even with small both δ and $\mathrm{Im}\tilde{\lambda}_{67}$.

Remark.—Note that in MSSM, etc. CP symmetry can be violated by interaction of Higgs fields with different scalar squarks, etc. In this case the mixed polarization operators $\mathrm{Im}\Pi_{HA}$ and $\mathrm{Im}\Pi_{hA}$ appear leading to the CP violation in the Higgs sector even for the CP-conserving Higgs potential. This violation can be visible if H and A or (and) h and A are almost degenerate (see e.g. [24] and references therein).

F. Couplings to gauge bosons

The gauge bosons V (W and Z) couple only to the CP-even fields η_1, η_2. For the physical Higgs bosons h_i (4.6) one obtains simple expressions for their couplings, which in terms of the relative couplings (1.3) read

$$\chi_V^{(i)} = \cos\beta R_{i1} + \sin\beta R_{i2}, \qquad V = W \text{ or } Z. \qquad (4.19a)$$

Note that due to unitarity of the transformation matrix R, the following sum rule takes place [25]:

$$\sum_{i=1}^{3} (\chi_V^{(i)})^2 = 1. \qquad (4.19b)$$

In particular, in the case of weak violation of the CP symmetry considered above, with s_2, s_3 given by Eqs. (4.18a), we obtain

$$\begin{aligned} \chi_V^{(1)} &= \sin(\beta-\alpha), \qquad \chi_V^{(2)} = -\cos(\beta-\alpha), \\ \chi_V^{(3)} &= -s_2\sin(\beta-\alpha) + s_3\cos(\beta-\alpha). \end{aligned} \qquad (4.20)$$

G. Higgs self-couplings

The decomposition of the scalar fields $\phi_{1,2}$ in terms of physical fields h_i allows us to identify the trilinear and quartic couplings among them via parameters of Lagrangian and elements of mixing matrix (4.7). They were obtained in [26–28]. For completeness, we present them for our specific form of Lagrangian (3.13) in the Appendix.

In the case of soft Z_2 symmetry violation in the CP conservation case these equations simplify, and we present in the Appendix self-couplings in this particular case as well.

For this very case we present two useful forms for trilinear couplings. First, we express these couplings in terms of masses and mixing angles α and β. Second, for the case of model II for Yukawa interaction (see below) we find expressions for these trilinear couplings in terms of masses and relative couplings to gauge bosons and quarks (and the parameter ν).

V. YUKAWA INTERACTIONS

A. General discussion

In the general case the Yukawa Lagrangian reads [10]

$$\begin{aligned} -\mathcal{L}_{\mathrm{Y}} = \bar{Q}_L[(\Gamma_1\phi_1 + \Gamma_2\phi_2)d_R \\ + (\Delta_1\tilde{\phi}_1 + \Delta_2\tilde{\phi}_2)u_R] + \text{H.c.}, \end{aligned} \qquad (5.1)$$

with similar terms for the leptons. Here, Q_L refers to the 3-family vector of the left-handed quark doublets, whereas d_R and u_R refer to the 3-family vectors of the right-handed field singlets (with $q_{\mathrm{L}} = (1-\gamma_5)q/2$ and $\tilde{\phi}_a = i\tau_2\phi_a^{*\mathrm{T}}$). The Yukawa matrices Γ and Δ are three-dimensional matrices in the family space with generally complex elements (Yukawa parameters).

Obviously the transformation (2.2) induces changes in the elements of matrices Γ_i and Δ_i. In particular, *the rephasing invariance* is extended to the full Higgs + Yukawa Lagrangian space if one supplements the transformations (2.5) of fields $\phi_{1,2}$ by the following transformations of fermion fields

$$Q_{Lk} \to Q_{Lk} e^{i\tau_{qk}}, \qquad d_{Rk} \to d_{Rk} e^{i(\tau_{qk}+\tau_{dk})}, \qquad u_{Rk} \to u_{Rk} e^{i(\tau_{qk}+\tau_{uk})}. \tag{5.2a}$$

The corresponding transformations of the parameters of Yukawa Lagrangian supplementing the transformations (2.6) are

$$\Gamma_1 \to \Gamma_1 \begin{pmatrix} e^{i\tau_{d1}} & & \\ & e^{i\tau_{d2}} & \\ & & e^{i\tau_{d3}} \end{pmatrix} e^{-i\rho_1}, \qquad \Delta_1 \to \Delta_1 \begin{pmatrix} e^{i\tau_{u1}} & & \\ & e^{i\tau_{u2}} & \\ & & e^{i\tau_{u3}} \end{pmatrix} e^{i\rho_1},$$
$$\Gamma_2 \to \Gamma_2 \begin{pmatrix} e^{i\tau_{d1}} & & \\ & e^{i\tau_{d2}} & \\ & & e^{i\tau_{d3}} \end{pmatrix} e^{-i\rho_2}, \qquad \Delta_2 \to \Delta_2 \begin{pmatrix} e^{i\tau_{u1}} & & \\ & e^{i\tau_{u2}} & \\ & & e^{i\tau_{u3}} \end{pmatrix} e^{i\rho_2}. \tag{5.2b}$$

An existence of the off-diagonal (in family index) terms in the Yukawa matrices results in the flavor-changing neutral currents. The rephasing invariance under the transformations (2.5) and (5.2b) allows to make real the diagonal elements of only one matrix Γ and one matrix Δ. Complex values of the other elements of matrices $\Gamma_{1,2}$ and $\Delta_{1,2}$ can result in the complex values of one-loop corrections to some λ's and in consequence to the *CP* violation in the Higgs sector discussed above (even for real bare coefficients m_{12}^2 and λ's). In the latter case, the corresponding *CP*-violating terms should be included in the Higgs Lagrangian in order to have a standard multiplicative renormalizability.

Note that in the case when simultaneously $\Gamma_1 \neq 0$ and $\Gamma_2 \neq 0$ or $\Delta_1 \neq 0$ and $\Delta_2 \neq 0$ (i.e. right-handed fermion of the type d_R or u_R interacts with both fields ϕ_1 and ϕ_2), the counterterms corresponding to the one-loop corrections to the Higgs Lagrangian contain operators of dimension 4, which violate Z_2 symmetry (1.2) in a hard way. They contribute to the renormalization of parameters $\varkappa$, λ_6, and λ_7 [11,20]. Therefore, to have only the soft violation of Z_2 symmetry (to prevent $\phi_1 \leftrightarrow \phi_2$ transitions at small distances), one demands that [4,29]

each right-handed fermion couples to only one scalar field, either ϕ_1 or ϕ_2. (5.3)

The case $\Gamma_2 = \Delta_1 = 0$ with diagonal Γ_1, Δ_2 corresponds to the well-known model II, while $\Gamma_2 = \Delta_2 = 0$—to the model I (see e.g. [1]). For the Lagrangian having simultaneously model II and soft Z_2 violated form these properties [vanishing $\lambda_6, \lambda_7, \varkappa = 0$ and (5.3)] are stable under the radiative corrections. Note that general RPaT makes these properties of Lagrangian hidden.

If for a given physical system both the model II (or model I) and the soft Z_2-violating Lagrangians exist but do not coincide, the radiative corrections transform a Lagrangian to that with a true hard violation of Z_2 symmetry. In this case only a general model like model III and with true hard violation of the Z_2 symmetry is renormalizable. We do not study this case since we consider it *unnatural*.

B. Model II

We limit ourselves to the case when the physical reality allows for the description of Higgs-fermion interaction in a form, where the fundamental scalar field ϕ_1 couples to d-type quarks and charged leptons ℓ, while ϕ_2 couples to u-type quarks (we take neutrinos to be massless)—the model II Lagrangians, which are represented by a crossed vertical strip in Fig. 1.

Using matrices $\Gamma_1 = \mathrm{diag}(g_{d1}, g_{d2}, g_{d3})$ and $\Delta_2 = \mathrm{diag}(g_{u1}, g_{u2}, g_{u3})$, we get

$$-\mathcal{L}_Y^{II} = \sum_{k=1,2,3} g_{dk} \bar{Q}_{Lk} \phi_1 d_{Rk} + \sum_{k=1,2,3} g_{uk} \bar{Q}_{Lk} \tilde{\phi}_2 u_{Rk} + \sum_{k=1,2,3} g_{\ell k} \bar{\ell}_{Lk} \phi_1 \ell_{Rk} + \mathrm{H.c.} \tag{5.4}$$

Certainly, the general RPaT (2.3) transforms Yukawa Lagrangian to a form where this basic definition of model II cannot be seen. These are *hidden model II forms of Lagrangian*. In entire reparameterization equivalent space these Lagrangians form a family shown by a crossed vertical strip in Fig. 1 (in this figure we suggest that this family coincides with soft Z_2 symmetry violated family).

The suitable choice of phases in transformations (2.6) and (5.2b) eliminates phase difference of vacuum expectation values and makes all Yukawa parameters real. It gives *a model II Lagrangian in a real vacuum form*. We will use such a Lagrangian below. It corresponds to the intersection of crossed and black strips in Fig. 1.

As it was written above, different forms of Lagrangian can have different values of $\tan\beta$. To underline that we use the mentioned Lagrangian, we will supply (only in this section) quantity β in this case by a subscript II, $\beta \to \beta_{II}$.

Since v.e.v.'s of scalar fields are responsible for the fermion mass similarly as in the SM, the relative Yukawa couplings of the physical neutral Higgs bosons h_i (1.3) are identical for all u-type and for all d-type quarks (and charged leptons). They can be expressed via elements of the rotation matrix R (4.6):

$$\chi_u^{(i)} = \frac{1}{\sin\beta_{II}}[R_{i2} - i\cos\beta_{II} R_{i3}], \qquad \chi_d^{(i)} = \frac{1}{\cos\beta_{II}}[R_{i1} - i\sin\beta_{II} R_{i3}]. \tag{5.5}$$

(Note that e.g. the interaction $\bar{d}_L(g_1 + ig_2)d_R$ + H.c. reads for the Dirac fermions as $\bar{d}(g_1 - i\gamma_5 g_2)d$.)

In the particular case of weak *CP* violation [with small s_2, s_3 (4.18)] these relative couplings, together with the

TABLE I. Basic relative couplings in the weak CP-violated 2HDM (II). In the upper lines results for the case with no CP violation and in lower lines the corresponding corrections $\propto s_2$, s_3 are presented.

	χ_V	χ_u	χ_d
h_1	$\sin(\beta_{II}-\alpha)\ (+0)$	$\frac{\cos\alpha}{\sin\beta_{II}}\ (-is_2\cot\beta_{II})$	$\frac{\cos\alpha}{\sin\beta_{II}}\ (-is_2\tan\beta_{II})$
h_2	$-\cos(\beta_{II}-\alpha)\ (+0)$	$-\frac{\sin\alpha}{\sin\beta_{II}}\ (-is_3\cot\beta_{II})$	$-\frac{\cos\alpha}{\cos\beta_{II}}(-is_3\tan\beta_{II})$
h_3	0 $(-s_2\sin(\beta_{II}-\alpha)+s_3\cos(\beta_{II}-\alpha))$	$-i\cot\beta_{II}$ $\left(-s_2\frac{\sin\alpha}{\sin\beta_{II}}+s_3\frac{\cos\alpha}{\sin\beta_{II}}\right)$	$-i\tan\beta_{II}$ $\left(+s_2\frac{\sin\alpha}{\cos\beta_{II}}+s_3\frac{\cos\alpha}{\cos\beta_{II}}\right)$

corresponding ones to gauge bosons, are presented in Table I.

For the interaction of the charged Higgs bosons e.g. with t quark, the Lagrangian (5.4) gives

$$\mathcal{L}_{H^-tb} = \frac{M_t}{v\sqrt{2}}\cot\beta_{II}\bar{b}(1+\gamma^5)H^-t + \frac{M_b}{v\sqrt{2}}\tan\beta_{II}\bar{b}(1-\gamma^5)H^-t + \text{H.c.} \quad (5.6)$$

In the cases of weak CP-violating and soft Z_2-violation the relative coupling of the neutral scalar h_i to the charged Higgs boson can be written as

$$\chi_{H^\pm}^{(i)} = \left(1-\frac{M_i^2}{2M_{H^\pm}^2}\right)\chi_V^{(i)} + \frac{M_i^2-\nu v^2}{2M_{H^\pm}^2}\,\text{Re}(\chi_u^{(i)}+\chi_d^{(i)}). \quad (5.7)$$

C. Set of useful relations in model II

The unitarity of the mixing matrix R allows us to obtain a number of relations [25,30,31] between the relative couplings of neutral Higgs particles to the gauge bosons (4.19a) and fermions (5.5) (*basic relative couplings*). Since such couplings can be treated as measurable quantities, relations between them are especially useful in phenomenological analyses.

Let us remind here that in these relations we use the quantity $\tan\beta_{II}$ which coincides with the ratio v_2/v_1 only for a model II Lagrangian (and does not have this simple sense for other forms of Lagrangian). It is described via the basic relative couplings for h_i as

$$\tan^2\beta_{II} = \frac{(\chi_V^{(i)}-\chi_d^{(i)})^*}{\chi_u^{(i)}-\chi_V^{(i)}} = \frac{1-|\chi_d^{(i)}|^2}{|\chi_u^{(i)}|^2-1} = \frac{\text{Im}\chi_d^{(i)}}{\text{Im}\chi_u^{(i)}}. \quad (5.8)$$

Certainly, these expressions hold also for h, H, A, except the last one, which is absent for h, H.

(1) *The pattern relation* among the basic relative couplings holds of *each neutral Higgs particle* h_i (in particular also for h, H, A in the case of CP conservation) [30,31]:

$$(\chi_u^{(i)}+\chi_d^{(i)})\chi_V^{(i)} = 1+\chi_u^{(i)}\chi_d^{(i)}, \quad \text{or} \quad (\chi_u^{(i)}-\chi_V^{(i)})(\chi_V^{(i)}-\chi_d^{(i)}) = 1-(\chi_V^{(i)})^2. \quad (5.9)$$

(2) *A vertical sum rule* for each basic relative coupling χ_j for *all three neutral Higgs bosons h_i is given by* [32]:

$$\sum_{i=1}^{3}(\chi_j^{(i)})^2 = 1 \qquad (j = V, d, u). \quad (5.10)$$

For couplings to the gauge bosons this sum rule, written also above in Eq. (4.19b), takes place independently on a particular form of the Yukawa interaction.

(3) The relations (5.5) allow us also to write for each neutral Higgs boson h_i *a horizontal sum rule* [32]:

$$|\chi_u^{(i)}|^2\sin^2\beta_{II} + |\chi_d^{(i)}|^2\cos^2\beta_{II} = 1. \quad (5.11)$$

These sum rules guarantee that the cross section to produce each neutral Higgs boson h_i (or h, H, A) of the 2HDM, in the processes involving Yukawa interaction, cannot be lower than that for the SM Higgs boson with the same mass [32].

(4) Besides, the useful *linear relation* follows directly from Eqs. (4.19a) and (5.5):

$$\chi_V^{(i)} = \cos^2\beta_{II}\chi_d^{(i)*} + \sin^2\beta_{II}\chi_u^{(i)} = \cos^2\beta_{II}\chi_d^{(i)} + \sin^2\beta_{II}\chi_u^{(i)*} \Rightarrow \begin{cases} \chi_V^{(i)} = \text{Re}(\cos^2\beta_{II}\chi_d^{(i)} + \sin^2\beta_{II}\chi_u^{(i)}), \\ \text{Im}(\cos^2\beta_{II}\chi_d^{(i)} - \sin^2\beta_{II}\chi_u^{(i)}) = 0. \end{cases} \quad (5.12)$$

(5) *The relation for CP violated parts of Yukawa couplings* is obtained by exclusion of β_{II} from the Eqs. (5.11) and (5.12)

$$(1-|\chi_d^{(i)}|^2)\,\text{Im}\chi_u^{(i)} + (1-|\chi_u^{(i)}|^2)\,\text{Im}\chi_d^{(i)} = 0. \quad (5.13)$$

1. Some applications

Remember that the relative couplings to quarks are generally complex in contrast to the couplings to gauge bosons. For h_i (or h, H, A) we found the following results:

From (5.11) we get

$$|\chi_u^{(i)}| \gg 1 \Rightarrow \tan\beta_{II} \ll 1; \qquad |\chi_d^{(i)}| \gg 1 \Rightarrow \tan\beta_{II} \gg 1. \tag{5.14}$$

It is instructive to consider now consequences of the relations (5.9)–(5.10) for the case when some basic relative couplings of a Higgs boson are close to ± 1.

In virtue of (5.11) we have for moderate $\tan\beta$

$$|\chi_u^{(i)}| \approx 1 \Rightarrow |\chi_d^{(i)}| \approx 1. \tag{5.15}$$

Note, that if $\tan\beta$ is extremely large or extremely small, *the horizontal sum rule* allows $|\chi_d^{(i)}|$ to differ strongly from 1 or $|\chi_u^{(i)}|$ to differ strongly from 1, respectively [in agreement with (5.14)].

Taking for definiteness the case of $\chi_j^{(2)} \approx \pm 1$, we get:

From (5.10),

$$\chi_u^{(2)} \approx \pm 1 \Rightarrow \chi_u^{(1)} \approx \pm i\chi_u^{(3)}, \qquad \chi_d^{(2)} \approx \pm 1 \Rightarrow \chi_d^{(1)} \approx \pm i\chi_d^{(3)}. \tag{5.16}$$

For $\chi_V^{(2)} \sim \pm 1$

$$\text{if } \chi_V^{(2)} \approx \pm 1 \Rightarrow \begin{cases} \text{(a)} & \chi_u^{(2)} \approx \chi_V^{(2)} \text{ or } \chi_d^{(2)} \approx \chi_V^{(2)}, \\ \text{(b)} & \chi_u^{(2)} \approx \chi_d^{(2)} \approx \chi_V^{(2)}, \\ \text{(c)} & \chi_V^{(1)} \approx \chi_V^{(3)} \approx 0, \\ \text{(d)} & \chi_u^{(1)}\chi_d^{(1)} \approx \chi_u^{(3)}\chi_d^{(3)} \approx -1. \end{cases} \tag{5.17}$$

The property (a) obtained from (5.8), means that the coupling of h_2 to at least one fermion type (u or d) is close to the $\chi_V^{(2)}$. The property (b) follows from property (a) and (5.12), at moderate $\tan\beta$. The fact that the couplings of Higgs bosons to gauge bosons are real leads, with the aid of (5.10), to the property (c). Taking into account property (c) and the pattern relation (5.8) we obtain property (d): the product of Yukawa couplings for other Higgs bosons (not h_2) is close to the corresponding product for pseudoscalar A in the CP-conserving case.

Certainly, results analogous to (5.16) and (5.17) hold in the cases when $\chi_j^{(1)} \approx \pm 1$ or $\chi_j^{(3)} \approx \pm 1$.

D. Comments on radiative corrections

All results described so far were obtained in the tree approximation. Let us discuss briefly the stability of relations (5.9)–(5.13) among in principle *measurable* parameters of the model in respect to the radiative corrections (RC) (treated mainly as the one-loop effects).

Certainly, the observable quantities correspond to the Lagrangian (and potential) with RC. Then one can treat the presented relations (5.9)-(5.13) as obtained from the renormalized parameters [the elements of mass-squared matrix $\mathcal{M}$, the v.e.v.'s ratio $\tan\beta$ (3.7b) and the corresponding Euler angles α_i of Eq. (4.7)].

The approach which we adopt in our analysis is to deal with *the relative couplings* (1.3)—the ratios of the couplings of each neutral Higgs boson h_i to the gauge bosons W or Z and to quarks or leptons ($j = W, Z, u, d, \ell \ldots$), to the corresponding SM couplings. We assume that for each such relative coupling the RC are included in both: the couplings of the 2HDM (in the numerator) and those of SM (in the denominator). The largest RC to the Yukawa $\phi\bar{q}q$ couplings are the one-loop QCD corrections due to the gluon exchange. They are identical in the SM and in the 2HDM and cancel in both ratios χ_u and χ_d. The same is valid for purely QED RC to all basic couplings as well as for electroweak corrections including virtual Z or W contributions.

The situation is different for the electroweak corrections containing Higgs bosons in the loops. They are different in the SM and 2HDM; moreover, their values depend on the parameters of 2HDM. These type of RC may modify slightly some relations presented in Sec. V. However, it is natural to expect that these RC are small (below 1%) except for some small corners of parameter space.

A delicate problem appears in a description of RC for the physical states after EWSB. The physical Higgs states become unstable and they have no asymptotic states. Therefore, the mass matrix, obtained from (4.5) with RC, and the scattering matrix, written in terms of these fields, become non-Hermitian. The effects of instability can be neglected when these Higgs bosons are almost stable (their widths are much smaller than the masses and mass splittings). These effects should be taken into account in the case of the approximate mass degeneracy, i.e. when some of masses M_i are very close to each other. In such case a good description of the masses and couplings is given by an approximation in which a (complex) matrix of polarization operators is added to the mass matrix (4.5). Full treatment of this problem demands a subtle theoretical analysis.

VI. CONSTRAINTS FOR HIGGS LAGRANGIAN

The parameters of Higgs potential are constrained by three types of conditions:

(i) positivity (vacuum stability) constraints
(ii) minimum constraints
(iii) tree-level unitarity and perturbativity constraints,

which we will discuss below. The positivity and unitarity constraints were discussed in literature till now only for the case of a soft Z_2 violation [33–37], and the unitarity constraints only in the *CP*-conserving case [38,39]. In the same case of soft Z_2 violation the latter constraints were extended to the *CP* nonconserving case in [33]. Here we present some new results for the case of hard Z_2 symmetry violation (see [7]).

A. Positivity (vacuum stability) constraints

To have a *stable vacuum*, the potential must be positive at large quasiclassical values of fields $|\phi_k|$ (*positivity constraints*) for an arbitrary direction in the (ϕ_1, ϕ_2) plane. These constraints were obtained for the case of soft Z_2 violation (see e.g. [33–37]). They are

$$\lambda_1 > 0, \qquad \lambda_2 > 0, \qquad \lambda_3 + \sqrt{\lambda_1\lambda_2} > 0, \\ \lambda_3 + \lambda_4 - |\lambda_5| + \sqrt{\lambda_1\lambda_2} > 0. \tag{6.1}$$

To obtain these constraints it is enough to consider only quartic terms of the potential. Let $(\phi_1^\dagger\phi_1) = x_1 \geq 0$, $(\phi_2^\dagger\phi_2) = x_2 \geq 0$. Then $(\phi_1^\dagger\phi_2) = \sqrt{x_1x_2}ce^{i\alpha}$ with $|c| \leq 1$ (due to Schwartz theorem). The quadratic form $V(x_1, x_2)$ should be positive at large x_i at different c and ϕ. At $x_2 = 0$ or x_1 we obtain two first conditions. At $c = 0$ the third inequality is derived. At $c = \pm 1$ with variation of α in respect to the phase of λ_5 we obtain the latter constraint.

B. Minimum constraints

The condition for vacuum (3.1) describes the *extremum* of potential but not obligatory the minimum. The *minimum constraints* are the conditions ensuring that the above extremum is a minimum for all directions in (ϕ_1, ϕ_2) space, except of the Goldstone modes (the physical fields provide the basis in the coset). This condition is realized if the mass matrix squared for the physical fields is positively defined, which means that its eigenvalues, i.e. the physical mass-squared, are positive: $M^2_{h_{1-3}}, M^2_{H^\pm} > 0$. In some applications the necessary conditions for that: positivity of all diagonal elements, principal minors, and the determinant of mass-squared matrix in different forms (4.5) or (4.15), are useful (see discussion in Sec. III).

C. Unitarity and perturbativity constraints

The quartic terms of Higgs potential (λ_i) are transformed to the quartic self-couplings of the physical Higgs bosons. They lead, in the tree approximation, to the *s*-wave Higgs-Higgs and W_LW_L and W_LH, etc. scattering amplitudes for different elastic channels. These amplitudes should not overcome unitary limit for this partial wave—that is *the tree-level unitarity constraint*.

The unitarity constraint was obtained first [4] in the frame of minimal SM, with one Higgs doublet and Higgs potential $V = (\lambda/2)(\phi^\dagger\phi - v^2/2)^2$ as the condition $3\lambda \leq 8\pi$. In this model the Higgs boson mass $M_H = v\sqrt{\lambda}$ and its width Γ_H, given mainly by a decay of Higgs boson to the longitudinal components of gauge bosons W_L, Z_L (originated from the Goldstone components $G^\pm$), grow with M_H as M_H^3. Therefore, the unitarity limit corresponds simultaneously to the case where $\Gamma_H \approx M_H$, so that the physical Higgs boson disappears. On the other hand it is well known that for $\lambda \gtrsim 8\pi$ at $\sqrt{s} > v\sqrt{\lambda} \gtrsim v\sqrt{8\pi} \approx 1.2$ TeV the Higgs boson self-interaction become strong; it is realized as a strong interaction of W_L and Z_L (appeared as Goldstone modes of a Higgs doublet at EWSB). Therefore, the unitarity limit is a boundary (in λ's space) between two different physical regimes. Below the unitarity limit we have a more or less narrow Higgs boson with well-known properties (and no strong interaction effects in the Higgs sector). Above the unitarity limit the Higgs boson disappears as a particle, discussion in terms of the observable Higgs particle becomes senseless, and the Higgs sector becomes strongly interacting.

Akeroyd *et al.* [39] have derived the unitarity constraints for the 2HDM without a hard violation of Z_2 symmetry for the *CP*-conserving case, i.e. for real λ_{1-5}. In the general *CP* nonconserving case with soft violation of Z_2 symmetry the parameter λ_5 is complex. The application of the RPhT (2.6) allows us to eliminate the phase of λ_5, coming to the rephasing equivalent Lagrangian with real $\lambda_5^s \equiv |\lambda_5|$ (m_{12}^2 remains complex). Use of this Lagrangian allows us to extend the results presented in [39] for unitary constraints to the *CP* nonconserving case [33].

In the considered cases the Z_2 symmetry is not violated by the quartic terms of potential. Unitarity constraints are written in Ref. [33] as the bounds for the eigenvalues $\Lambda_{Y\sigma}^{Z_2\text{parity}}$ of the high energy Higgs-Higgs scattering matrix for the different quantum numbers of an initial state: total hypercharge Y, weak isospin σ, and Z_2 parity. These bounds given separately for the Z_2-even ($\phi_1\phi_1$ and $\phi_2\phi_2$) and Z_2-odd ($\phi_1\phi_2$) initial states are as follows:

$$|\Lambda_{Y\sigma\pm}^{Z_2}| < 8\pi \quad \text{with}$$
$$\Lambda_{21\pm}^{\text{even}} = \frac{1}{2}(\lambda_1 + \lambda_2 \pm \sqrt{(\lambda_1 - \lambda_2)^2 + 4|\lambda_5|^2}),$$
$$\Lambda_{21}^{\text{odd}} = \lambda_3 + \lambda_4, \qquad \Lambda_{20}^{\text{odd}} = \lambda_3 - \lambda_4,$$
$$\Lambda_{01\pm}^{\text{even}} = \frac{1}{2}(\lambda_1 + \lambda_2 \pm \sqrt{(\lambda_1 - \lambda_2)^2 + 4\lambda_4^2}),$$
$$\Lambda_{01\pm}^{\text{odd}} = \lambda_3 \pm |\lambda_5|,$$
$$\Lambda_{00\pm}^{\text{even}} = \frac{3(\lambda_1 + \lambda_2) \pm \sqrt{9(\lambda_1 - \lambda_2)^2 + 4(2\lambda_3 + \lambda_4)^2}}{2},$$
$$\Lambda_{00\pm}^{\text{odd}} = \lambda_3 + 2\lambda_4 \pm 3|\lambda_5|. \tag{6.2}$$

For real λ_5 these conditions coincide with those from [39], obtained however without the above mentioned identification of various contributions.

At small ν these constraints result in a moderately large upper bound of $600 \div 700$ GeV for M_H, M_A, $M_{H^\pm}$ (see examples in Table II of Sec. VII B), see also e.g. [39] for the CP-conserving case. At large ν, all Higgs bosons except h_1 become heavy without violating of the unitary constraints (6.2).

The correspondence between a violation of the tree-level unitarity limit and a lack of realization of the Higgs field as a resonance (a particle), as in the minimal SM, takes place in the 2HDM only in the case when *all* constraints (6.2) are violated simultaneously. In the case when only some of these constraints are violated the physical picture becomes more complex. One can imagine, for example, a situation when some of the Higgs bosons are "normal" scalars, i.e. their properties can be estimated perturbatively, while the others interact strongly at sufficiently high energy. In such case, the unitarity constraints work differently for different *physical* channels, in particular, for different Higgs bosons.

The *perturbativity condition (constraint)* for a validity of a tree approximation in the description of some particular phenomena (e.g. interactions of the lightest Higgs boson h_1) may be less restrictive than the presented above general unitarity constraints. The explicit form of the perturbativity constraint should be found;, however, this is a subject for a separate consideration. In particular, the effective parameters of perturbation theory for the Yukawa interaction is $g^2/(4\pi)^2$. Therefore, one of the necessary conditions for the smallness of radiative corrections is $|g| \ll 4\pi$.

D. The case of hard Z_2 violation

The analysis of the case with hard Z_2 violation (i.e. the potential with $\lambda_{6,7}$ terms) is more complicated. One can say definitely that the positivity constraints (6.1) are valid for some particular directions of a growth of the quasiclassic fields $\phi_{1,2}$. Similarly, unitarity constraints (6.2) hold for such transition amplitudes which do not violate the Z_2 symmetry.

For the hard violation of Z_2 symmetry one should consider new directions in the (ϕ_1, ϕ_2) space which appear due to λ_6, λ_7 terms and the processes like $\phi_1\phi_1 \to \phi_1\phi_2$, which violate the Z_2 symmetry. Therefore the new positivity and unitarity constraints should include parameters λ_6, λ_7. In any case conditions (6.2) are necessary for unitarity [7].

VII. HEAVY HIGGS BOSONS IN 2HDM

Many analyses of 2HDM assume a SM-like physical picture: the lightest Higgs boson h_1 is similar to the Higgs boson of the SM while other Higgs bosons escape observation being too heavy. Besides, many authors assume *in addition* that masses of other Higgs bosons M are close to the scale of new physics, $M \sim \Lambda$, and that the theory should possess an explicit *decoupling property*[4], i.e. *the correct description of the observable phenomena must be valid for the (unphysical) limit* $M \to \infty$ [37,41–44]. However, the 2HDM allows also for another realization of the mentioned SM-like physical picture.

Looking on formulas from Sec. IV we see that the large masses of Higgs particles may arise from large parameters ν or $\lambda' s$, or both. Obviously, large values of $\lambda' s$ may be in conflict with unitarity constraints, which is not the case for large ν. Below we discuss these two very distinct sources of large masses, and their different phenomenological consequences.

A. Decoupling of heavy Higgs bosons

In 2HDM the decoupling case corresponds to

$$\nu \gg |\lambda_i|. \tag{7.1}$$

(It cannot be realized for the exact Z_2 symmetry.) In this case equations for masses and mixing angles α_i (4.13) simplify. First we find, with accuracy up to the λ/ν terms, masses of the subsidiary Higgs states obtained at the first stage of diagonalization (4.9)–(4.14). From Eqs. (4.12) we derive

$$\begin{aligned}\frac{M_h^2}{v^2} &= \underbrace{c_\beta^4\lambda_1 + s_\beta^4\lambda_2 + 2s_\beta^2c_\beta^2\lambda_{345}}_{\text{soft}} + \underbrace{4s_\beta^2c_\beta^2\,\mathrm{Re}\lambda_{67}}_{\text{hard}},\\ \frac{M_H^2}{v^2} &= \underbrace{\nu + s_\beta^2c_\beta^2(\lambda_1 + \lambda_2 - 2\lambda_{345})}_{\text{soft}}\\ &\quad - \underbrace{[(c_\beta^2 - s_\beta^2)\,\mathrm{Re}\tilde{\lambda}_{67} + (4s_\beta^2c_\beta^2 - 1/2)\,\mathrm{Re}\lambda_{67}]}_{\text{hard}}.\end{aligned} \tag{7.2}$$

At $\nu \to \infty$ we have $\beta - \alpha \to \pi/2$. It is useful to characterize a deviation from this value by a parameter $\Delta_{\beta\alpha} = \pi/2 - (\beta - \alpha)$. Using $s_{2\beta} = \sin 2\beta$, $c_{2\beta} = \cos 2\beta$, we get from the second line of Eq. (4.13):

$$\begin{aligned}\Delta_{\beta\alpha} &= -\frac{L_a s_{2\beta}}{2\nu},\\ L_a &= \underbrace{s_\beta^2\lambda_2 - c_\beta^2\lambda_1 + c_{2\beta}\lambda_{345}}_{\text{soft}} + \underbrace{\mathrm{Re}(2c_{2\beta}\lambda_{67} - \tilde{\lambda}_{67})}_{\text{hard}}.\end{aligned} \tag{7.3}$$

The subsequent complete diagonalization, described in Sec. IV D, is simplified by condition (7.1). We get the following results:

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[4]Generally, this property is an important feature of any consistent theory describing phenomena at some distances (energies), that is an independence of its predictions from the dynamics at smaller distances, described by some mass scale M [40].

1. The lightest Higgs boson h_1

The Eqs. (4.14), (3.11) show that under the condition (7.1) the element M'_{13} of the matrix (4.9), responsible for the mixing of scalar h with A, is small as compared to the mass difference $M_A^2 - M_h^2 \approx \nu v^2$. Therefore, the state h_1 is very close to h. The mixing angle α_2, describing the CP-odd admixture in this state, is given by $s_2 \sim |\lambda|/\nu (\ll 1)$ (4.18a). The shift of the mass of h_1 from the M_h value (7.2) is given by Eq. (4.18c), i.e. $M_1^2 - M_h^2 \sim |\lambda|/\nu$, and can be neglected.

Since for $\nu \to \infty$ the $\Delta_{\beta\alpha} \to 0$ the scalar h_1 couples to the gauge bosons and to the quarks and leptons in the model II as in the SM (with accuracy $|\lambda|/\nu$) even for the general CP nonconserving case. Besides, h_1 practically decouples from $H^\pm$, since the quantity $\chi_{H^\pm}^{(1)} \sim \mathcal{O}(|\lambda|/\nu)$ (5.7).

2. Higgs bosons h_2, h_3, and $H^\pm$

The Eqs. (4.3), (4.5c), and (7.2) show that

$$M_{H^\pm}^2 \approx M_A^2 \approx M_H^2 = v^2\nu\left[1 + \mathcal{O}\left(\frac{|\lambda|}{\nu}\right)\right], \tag{7.4a}$$

i.e. $H^\pm$, H, and A are very heavy and almost degenerate in masses, and similarly for h_2 and h_3

$$M_{H^\pm}^2 \approx M_2^2 \approx M_3^2 \approx v^2\nu\left[1 + \mathcal{O}\left(\frac{|\lambda|}{\nu}\right)\right]. \tag{7.4b}$$

That is one of the reasons to consider the condition of the decoupling regime (7.1) in the form, used e.g. in Ref. [37],

$$M_A^2 \gg |\lambda| v^2. \tag{7.5}$$

In the considered case the CP-violating mixing between H and A can be strong, i.e. mixing angle α_3 given by Eq. (4.17a), can be large as it was discussed in Sec. IV E.

Since $\chi_V^{(h)} \approx 1$, the coupling of H to gauge bosons is very small, while A does not couple to gauge bosons (Table I). With mixing between H and A states given by angle α_3, we have

$$\chi_V^{(H)} = \cos(\beta - \alpha) \approx \Delta_{\beta\alpha},$$
$$\chi_V^{(A)} = 0 \Rightarrow \chi_V^{(2)} \approx -\cos\alpha_3 \Delta_{\beta\alpha}, \qquad \chi_V^{(3)} \approx \sin\alpha_3 \Delta_{\beta\alpha}. \tag{7.6a}$$

Besides, the couplings of H and A to the u-type fermions coincide in their modules (see Table I) (and the same is valid for d-type fermions and charged leptons), so that also the corresponding couplings of $h_{2,3}$ have equal modules, while their phases, related to the CP violation in the $(\bar{u}h_{2,3}u)$ and $(\bar{d}h_{2,3}d)$ vertices, are given by the mixing angle α_3. Using Eqs. (5.5) and (4.7) we obtain

$$\chi_u^{(2)} = i\chi_u^{(3)} = \cot\beta e^{-i\alpha_3},$$
$$\chi_d^{(2)} = -i\chi_d^{(3)} = -\tan\beta e^{i\alpha_3}. \tag{7.6b}$$

The corresponding Higgs decay widths are given mainly by the fermionic contributions,

$$\Gamma_H \approx \Gamma_A \approx \Gamma_2 \approx \Gamma_3 = \frac{3}{16\pi}\cot^2\beta\left[1 + \frac{m_b^2}{m_t^2}\tan^4\beta\right]M_H, \tag{7.6c}$$

$(\Gamma_A - \Gamma_H)/\Gamma_H \sim m_t/M_H$. (Here we took into account that $v^2/m_t^2 \approx 2$.) The gauge boson contributions to these widths are negligibly small $(\sim L_a^2/\nu)$. Therefore, we have $|M_H^2 - M_A|^2 \lesssim \Gamma_A M_A, \Gamma_H M_H$ at very large ν. In this case the equations for α_3, $M_{2,3}$, and $\Gamma_{2,3}$ become more complex, since they include shift of the A, H poles due to their proper widths (7.6c). The obtained mass matrix becomes non-Hermitian, therefore, the mixing angle α_3 becomes complex, and states h_2, h_3 become nonorthogonal. It is seen from Eq. (4.17), corrected for these effects:

$$\tan 2\alpha_3 \approx \frac{2M'_{23}}{M_A^2 - M_H^2 - i(M_A\Gamma_A - M_H\Gamma_H)} \tag{7.7}$$

(see [14,45] for more details of mixing). In this case Eqs. (7.6b) are modified.

Note that with this strong overlapping of states experimental distinguishing of states h_2, h_3 may be difficult. The visible effects of CP violation in the fermion interaction (like spin correlations, etc.) will be very similar in two quite different cases: of a true CP violation and of a strong overlapping of H and A states without the CP-violating mixing.

B. Heavy Higgs bosons without decoupling

The option, where except of one neutral Higgs boson h_1 (or h), all other Higgs bosons are reasonably heavy, can also be realized in 2HDM for a relatively small ν, i.e. beyond the decoupling limit. In this case possible masses of heavy Higgses are bounded from above by the unitarity constraints for λ_i, discussed in Sec. VI C. These constraints obtained for the CP-conserving case [39] can be generally stronger in the case of CP violation, since the constraints (6.2) puts limit on parameter $|\lambda_5|$ while formulas for masses contain solely $\mathrm{Re}\lambda_5$. In the Table II we present some particular examples of sets of parameters of the potential for light h (mass 120 GeV) and heavy H, $H^\pm$ for a nondecoupling case (small ν) and satisfying unitarity constraints (6.2).

The first three lines contain sets of parameters λ_i and ν for the case without CP violation with reasonably heavy H, $H^\pm$, A. One sees that these masses can be obtained for very large or very small $\tan\beta$ and reasonably small $\nu \approx (M_h/v)^2$, as well as for $\tan\beta \approx 1$ with $\nu \approx 0$.

The fourth line of the Table II presents an example of the *natural set of parameters* (see below), with heavy H and $H^\pm$ in the weak CP violation case. Since here mixing angles α_2, α_3 are small, the physical states h_1, h_2, h_3 are

TABLE II. Sets of parameters of potential for light h (mass of 120 GeV) and heavy H, $H^{\pm}$ satisfying unitarity constraints in the nondecoupling case.

$\tan\beta$	λ_1	λ_2	λ_3	λ_4	λ_5	ν	M_h	M_H	M_A	$M_{H^{\pm}}$	s_2	s_3
50	1	6	5.5	-6	-6	0.24	120	600	600	600	0	0
0.02	6	1	5.5	-6	-6	0.24	120	600	600	600	0	0
1	6.25	6.25	6.25	-6	-6	0	120	600	600	600	0	0
10	4	8	4.4	-9	$-0.5 + 0.3i$	0.24	120	700	206	556	0.09	0.02

close to the states h, $-H$ and A, existing in the CP conserved case.

In the considered nondecoupling case couplings of the lightest Higgs boson to the gauge bosons, quarks and leptons can be either close to the corresponding SM values (as in the decoupling case) or far from these values. The case when all basic couplings of the lightest Higgs boson are close to those of SM Higgs boson is discussed in detail in paper [46], see also [30,31]. Note, that even in such cases some nondecoupling effects due to heavy Higgs bosons may appear, e.g. $\chi_{H^{\pm}}^{(1)} \sim 1$, in contrast to the decoupling limit, discussed in Sec. VII A, where $\chi_{H^{\pm}}^{(1)} \sim 0$. It is worth noticing that ν parameter can be negative, which is not possible in the decoupling limit.

C. A natural set of parameters of 2HDM

It is natural to consider 2HDM as low energy approximation of some more general theory operating at smaller distances. In such theory fields ϕ_1 and ϕ_2 should differ in some quantum numbers which cannot be seen at our relatively large distances (like in MSSM). Therefore, it is natural to assume that the 2HDM describing physical reality allows an existence among the reparameterization equivalent Lagrangians the one in which fields ϕ_k do not mix at small distances (mixed kinetic term does not appear). That is the 2HDM with exact or softly violated Z_2 symmetry. We assume such choice in this section.

Besides, it is naturally to assume that the CP symmetry in the Higgs sector is violated only weakly at least for the lightest Higgs boson h_1. This assumption together with rephasing invariance offers the basis for the selection of the *natural set of parameters of 2HDM*.

The Eq. (4.9) shows that the CP symmetry for the lightest Higgs boson is violated weakly if and only if $|M'_{13}| \ll |M_A^2 - M_h^2|$. In view of (4.14), for *the real vacuum Lagrangian* at $\beta + \alpha \neq \pi/2$ this condition can be rewritten in the form

$$v^2|\mathrm{Im}m_{12}^2| \ll v_1 v_2 |M_A^2 - M_h^2|. \qquad (7.8)$$

For all other rephasing equivalent Lagrangians the condition corresponding to the Eq. (7.8) contains both $\mathrm{Im}m_{12}^2$ and $\mathrm{Re}m_{12}^2$. Therefore, for *the natural set of parameters of 2HDM* we require that both $|\mathrm{Im}m_{12}^2|(v^2/v_1v_2)$ and $|\mathrm{Re}m_{12}^2|(v^2/v_1v_2)$ are small for all rephasing equivalent Lagrangians. In virtue of (3.10) and (3.11) in the case of soft violation of Z_2 symmetry the same requirement is transmitted to $\mathrm{Im}\lambda_5$ and $\mathrm{Re}\lambda_5$. Therefore, we define *a natural set of parameters* as follows:

$$|\nu|, |\lambda_5| \ll |\lambda_{1-4}|. \qquad (7.9)$$

On the contrary, in the decoupling case, the term m_{12}^2 has the *unnatural property* $\mathrm{Re}m_{12}^2 \gg |\mathrm{Im}m_{12}^2|$. From this point of view *the decoupling case of 2HDM* (7.1) *is unnatural.*

For the natural set of parameters of 2HDM the breaking of the Z_2 symmetry is governed by a small parameter ν. Because of the existence of a limit when Z_2 symmetry holds, a small soft Z_2 violation in the Higgs Lagrangian and the Yukawa interaction remains small also beyond the tree level. In this respect we use the term *natural* in the same sense as in Ref. [5]. (Note that also nondiagonal Yukawa coupling matrices Γ_1 and Δ_2 (leading to FCNC) are unnatural in this very sense).

In accordance with Eq. (4.5), for the natural set of parameters also M_A cannot be too large (see Table II). This opportunity is not ruled out by data, see for CP-conserving case e. g. [47].

Remark on Yukawa sector.—In the case of true hard violation of Z_2 symmetry the Yukawa sector cannot be described by a simple model of type I or II, i.e. models like model III should be realized. However in such models the FCNC effects (and CP violation in the Higgs sector) are naturally large. That is an additional reason why the natural set of parameters of 2HDM corresponds to the case of exact or softly violated Z_2 symmetry with the model II or model I for Yukawa interaction.

VIII. SUMMARY AND DISCUSSION OF RESULTS

In this paper we analyze various aspects of the two-Higgs-doublet extension of the SM from the point of view of its symmetries. We critically discuss the standard formulations as well as applications of the 2HDM. Let us describe our approach and summarize main results and observations presented in the paper.

At the beginning we stress that the CP violation can be implemented in a model in a few different ways. In this paper we consider mainly the CP violation governed by complex parameters of the Higgs Lagrangian. However, there are other ways of implementation of CP violation. For example the one mentioned in Sec. VA, which relies on complex elements of the Yukawa matrices. Another way, used in fact in many analyses of MSSM, is based on the *CP* nonconservation in the couplings of Higgs bosons to superpartners. The renormalizability demands to add in such cases the *CP*-violating terms also in the Higgs Lagrangian.

In the analysis of symmetry properties of the model we introduce *the 16-dimensional space of Higgs Lagrangians with coordinates given by the Lagrangian parameters*. Within this space there is the three-dimensional subspace—*the reparameterization equivalent subspace*, formed by Lagrangians which can be obtained from a chosen one by the reparameterization transformation RPaT's (2.3). All the Lagrangians from this subspace describe the same physical reality (a reparameterization invariance). Different properties of the physical model can either be explicit or hidden for the different Lagrangians in the mentioned reparameterization equivalent subspace. Accordingly, different families of these Lagrangians are suitable for the study of different properties of the model. Obviously, all measurable quantities characterizing a system (like the coupling constants and masses) are reparameterization invariant while many other parameters of theory (like $\tan\beta$) are reparameterization dependent.

Certainly the concept of the reparameterization invariance, etc. can be easily generalized to a description of other models, e.g. with three or more Higgs doublets sector, etc. and for description of Yukawa interactions.

The reparameterization equivalent space is naturally sliced to *the rephasing equivalent subspaces*, which are described by transformations (2.2) with $\theta = 0$ (the RPhT's) represented by vertical strips in Fig. 1. One can characterize these subspaces e.g. by the value of ratio of v.e.v.'s $tan\beta$.

The *CP* violation in the Higgs sector means that the physical neutral Higgs bosons have no definite *CP* parity. The necessary condition for such *CP* violation is that some coefficients of the Higgs Lagrangian are complex. However, complex parameters can appear also in the *CP*-conserving case if the pertinent form of Lagrangian is not chosen. We found a specific, *real vacuum form of a Lagrangian* in which complexity of the parameters of Higgs Lagrangian becomes a sufficient condition for the *CP* violation in the Higgs sector. For the arbitrary form of Lagrangian we give a simple necessary and sufficient condition for the *CP* violation in the Higgs sector (4.8). This condition is simpler to use than a similar condition written via IRpaT in Ref. [8].

Some authors consider also the case when basic Higgs Lagrangians give no *CP* violation in the Higgs sector but this violation appears through the Yukawa interaction. The series of combination of Higgs self-couplings and Yukawa couplings form reparameterization independent invariants, describing condition for the *CP* violation. Note that in this case loop corrections from the Yukawa interaction produce *CP* violated terms in the Higgs Lagrangian. From general renormalizability such terms must be included in the basic Higgs Lagrangian and our simple criteria for *CP* violation (4.16) seem to be sufficient.

The 2HDM provides the mechanism of the EWSB which allows for potentially large *CP* violation and FCNC effects. These phenomena are controlled to a large extent by the Z_2 symmetry under transformation (1.2) of the Lagrangian and various degrees of its violation. If the Z_2 invariance holds, then the considered doublets of scalar fields $\phi_{1,2}$ are the true fundamental basic fields before EWSB. The soft violation of Z_2 symmetry is given by the mixed mass term $\sim m_{12}^2$ in the Higgs potential. In this case two doublets $\phi_{1,2}$ mix near the EWSB scale but they do not mix at sufficiently small distances. The RPaT converts such Higgs Lagrangian, $\mathcal{L}_s$, to the form with terms typical for a hard violation of the Z_2 symmetry (*a hidden soft Z_2 violation form of Lagrangian*). However, in this case the parameters of the Higgs potential are interrelated as it is given by Eq. (2.7) [see also Eqs. (2.8)]. It prevents an appearance of a running coefficient at the mixed kinetic term.

In the case of true hard violation of Z_2 symmetry even the discussion of Higgs potential alone is incomplete, since it is necessary to consider more general Higgs Lagrangian with the mixed kinetic term. The coefficient of this mixed term of Lagrangian $\varkappa$ (2.1b) generally runs due to the loop corrections. At some fixed distance (renormalization scale) the kinetic part of the Lagrangian can be removed by diagonalization like (2.9) but this term is restored at other distances (renormalization scales) due to the loop corrections from hard terms of the Higgs potential. We did not find a fully consistent formulation of 2HDM in the case when the mixed kinetic term is present. We argue, that due to the mentioned relation to the phenomena at small distances, the case with soft violation of Z_2 symmetry looks much more attractive and natural.

In our calculation we keep separately contributions of soft and hard violations of Z_2 symmetry. Nevertheless, our discussion of a hard violation of Z_2 symmetry is as incomplete as all other existing analyses, since effects related to the running coefficient of the mixed kinetic term should be analyzed in addition.

The EWSB appears at the minimization of a Higgs potential giving the vacuum expectation values for two scalar fields, ϕ_1 and ϕ_2.For some set of parameters of Lagrangian these v.e.v.'s describe a standard (neutral) vacuum. Generally, phases of these v.e.v.'s differ from each other. However, this phase difference can be eliminated by a suitable rephasing transformation giving the mentioned above real vacuum Lagrangian. We prefer to express the mass coefficients of Higgs potential via $v_{1,2}$ and the free dimensionless parameter $\nu \propto \mathrm{Re}m_{12}^2$, (3.10). We use in our analysis such forms of Lagrangians.

For other sets of parameters of Lagrangian the condition of minimum of the potential defines also exotic "charged vacuum'' with vacuum energy larger than that for the standard vacuum [15,16].

Some physical model (''physical reality'') is described by many reparameterization equivalent Lagrangians. On the contrary, the description of Lagrangian in terms of the observable Higgs fields h_i is unique (reparameterization invariant). For the neutral Higgs sector the transition from fields ϕ_1 and ϕ_2 to the basis of observable Higgs bosons is rather complicated. We have performed this in two steps. First, we diagonalize the CP-even part of the mass-squared matrix. For the Lagrangian in a real vacuum form this step is identical to the one used in the CP-conserving case. It allows us to describe the general CP-violating case in terms of the well-known states h, H, and A treated now as the subsidiary states (i.e. having no direct physical meaning). Using these states it becomes evident that the existence of complex coefficients in the Higgs potential in a real vacuum form is a necessary and sufficient condition for the CP violation in the Higgs sector. Our procedure allows us to analyze easily various important cases when one of neutral Higgs boson is almost the CP-even one, while two other neutral Higgs bosons strongly mix, i.e. CP symmetry can be strongly broken in the processes with exchange of these Higgs bosons.

Considering the Yukawa interactions we note that for a case of true hard violation of Z_2 symmetry the most general form of this interaction (e.g. model III) should be implemented. However, we limit ourselves to models in which each fermion isosinglet couples to only one Higgs field and discuss the flavor structure of such couplings. We consider in detail the model II. We assume that the model II Lagrangian family coincides with the above mentioned family of Lagrangians with explicit softly violated Z_2 symmetry. We prefer to use the Lagrangian in the form which corresponds to the real vacuum, model II and exact or softly violated Z_2 symmetry in the potential.

In this paper we extend our approach introduced earlier for the CP-conserving case in [30,31] to the analysis of the CP nonconserving case. This approach relies on using the measurable (in principle) Higgs boson masses and basic relative couplings (1.3) plus parameter ν (3.10) instead of variety of parameters λ and mixing angles α_i, β. This way phenomenological analyses become more transparent.

We present a series of relations between different relative couplings of each Higgs boson, (5.9)–(5.13). Among these relations there are well-known sum rules, the pattern relation (obtained by us in [30] for the CP-conserving case and in [31] for the CP violation), new linear relations and their combinations. Equation (5.8) represents the formulas which allow us to determine the quantity $\tan\beta$ for the Lagrangian in model II form, $\tan\beta_{II}$.

Using these relations we obtained various useful relations among couplings of Higgs bosons to quarks and gauge bosons in the case when some of these couplings (or their absolute values) are close to the corresponding values in the SM (5.14)–(5.17).

As the mentioned relations between relative couplings are of great phenomenological importance it was crucial to check how the radiative corrections influence them; we argue that radiative corrections change only weakly the considered relations.

Next we combine and discuss different types of constraints on the parameters of the Higgs potential (the positivity condition or—in other words—the vacuum stability condition at large quasiclassical values of ϕ_k, the existence of a minimum, the tree-level unitarity constraint from the Higgs-Higgs scattering matrix) both in the CP-conserving and CP-violating cases. Some of them were known until now only in the CP-conserving case. All known results were obtained for the case of soft violation of Z_2 symmetry only. We ascertained that some of these results are valid also in the case of hard violation of Z_2 symmetry, as a part of a more general system of constraints.

We perform the detailed discussion on an opportunity that in the 2HDM there is one light Higgs boson, while others are much heavier, so that they can escape observation. As it was already claimed in [31,37], such a situation can be realized in the different regions of ν. At $\nu \gg |\lambda_i|$ we have decoupling case in which the lightest Higgs bososn h_1 is very similar to the SM Higgs boson, while other Higgs bosons except h_1 are very heavy and almost degenerate in masses. We found simple expressions for their couplings which hold for a possible strong CP-violating mixing among them (7.6).

At small ν, the reasonably heavy Higgs bosons, lighter however than ~600 GeV, may appear without violation of unitarity constraints. This small ν option looks more natural from the point of view of the rephasing invariance. Here one can expect some nondecoupling effects due to the heavy Higgs bosons [30,31,48]. The detailed analysis of various SM-like realizations and some nondecoupling effects is presented in [46].

In the Appendix we present for completeness a whole set of self-couplings of physical Higgs bosons in the general CP-violating case. In addition, we present simple formulas for the CP-conserving, soft Z_2-violating case. In addition to the well-known forms of these couplings, for the case when the Yukawa interaction is described by model II, we express all trilinear couplings via the Higgs masses and their relative couplings to the gauge bosons and fermions of the physical Higgs bosons entering corresponding vertex and the parameter ν.

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APPENDIX A: HIGGS SELF-COUPLINGS

The fact that the charged Higgs field $H^\pm$ and axial field A are expressed via fields ϕ_k and angle β allows us to obtain Higgs self-couplings in a two-step procedure. At the first step we come to basis η_1, η_2, $H^\pm$, A (4.1)–(4.4). Then we perform transformation (4.7). It results in the appearance of a suitable number of matrix elements R_{ij} in addition to factors b_A or a_A [Eqs. (A1) and (A2)], which are expressed via couplings λ_i, given in the real vacuum form, and mixing angle β. In the equations below the symbol $*$ denotes a sum over permutations over summation indices i, j, etc. (giving factors of $n!$ for n identical indices).

For the couplings involving the charged Higgs bosons we have

$$\begin{aligned} g_{h_i H^+ H^-} &= v \sum_{m=1,2,3} R_{im} b_m, \\ g_{h_i h_j H^+ H^-} &= \sum_{m\le n=1,2,3}^{*} R_{i'm} R_{j'n} b_{mn}, \\ g_{H^+H^-H^+H^-} &= 2[\sin^4\beta\lambda_1 + \cos^4\beta\lambda_2 \\ &\quad + 2\cos^2\beta\sin^2\beta\,\mathrm{Re}\lambda_{345} \\ &\quad - 4\cos\beta\sin\beta(\sin^2\beta\,\mathrm{Re}\lambda_6 + \cos^2\beta\,\mathrm{Re}\lambda_7)]. \end{aligned} \tag{A1}$$

For the couplings among the neutrals we have

$$\begin{aligned} g_{h_i h_j h_k} &= v \sum^{*} R_{i'm} R_{j'n} R_{k'o} a_{mno}, \\ g_{h_i h_j h_k h_l} &= \sum^{*} R_{i'm} R_{j'n} R_{k'o} R_{l'p} a_{mnop}, \end{aligned} \tag{A2}$$

with $m \le n \le o \le p = 1, 2, 3$.

The coefficients b_m, b_{mn}, a_{mno}, a_{mnop} presented below agree with the corresponding results of [26–28].

1. General formulas

a. Trilinear couplings

The trilinear couplings involving the charged Higgs bosons are given by Eq. (A1), with

$$\begin{aligned} b_1 &= \cos\beta\{\sin^2\beta(\lambda_1 - \lambda_{345}) + \lambda_3 \\ &\quad + \cos\beta\sin\beta[(\tan^2\beta - 2)\,\mathrm{Re}\lambda_6 + \mathrm{Re}\lambda_7]\}, \\ b_2 &= \sin\beta\{\cos^2\beta(\lambda_2 - \lambda_{345}) + \lambda_3 \\ &\quad + \cos\beta\sin\beta[\mathrm{Re}\lambda_6 + (\cot^2\beta - 2)\,\mathrm{Re}\lambda_7]\}, \\ b_3 &= \cos\beta\sin\beta\,\mathrm{Im}\lambda_5 - \sin^2\beta\,\mathrm{Im}\lambda_6 - \cos^2\beta\,\mathrm{Im}\lambda_7. \end{aligned} \tag{A3}$$

The trilinear couplings among neutral Higgs fields are given by Eq. (A2), where:

$$\begin{aligned} &a_{111} = \tfrac{1}{2}(\cos\beta\lambda_1 + \sin\beta\,\mathrm{Re}\lambda_6), \qquad a_{112} = \tfrac{1}{2}(\sin\beta\,\mathrm{Re}\lambda_{345} + 3\cos\beta\,\mathrm{Re}\lambda_6), \\ &a_{113} = -\tfrac{1}{2}[\cos\beta\sin\beta\,\mathrm{Im}\lambda_5 + (1 + 2\cos^2\beta)\,\mathrm{Im}\lambda_6], \qquad a_{122} = \tfrac{1}{2}(\cos\beta\,\mathrm{Re}\lambda_{345} + 3\sin\beta\,\mathrm{Re}\lambda_7), \\ &a_{123} = -\mathrm{Im}\lambda_5 - \cos\beta\sin\beta(\mathrm{Im}\lambda_6 + \mathrm{Im}\lambda_7), \\ &a_{133} = \tfrac{1}{2}\{\cos\beta(\sin^2\beta\lambda_1 + \cos^2\beta\,\mathrm{Re}\lambda_{345} - 2\,\mathrm{Re}\lambda_5) + \sin\beta[\sin^2\beta\,\mathrm{Re}\lambda_6 + \cos^2\beta\,\mathrm{Re}(\lambda_7 - 2\lambda_6)]\}, \\ &a_{222} = \tfrac{1}{2}(\sin\beta\lambda_2 + \cos\beta\,\mathrm{Re}\lambda_7), \qquad a_{223} = -\tfrac{1}{2}[\cos\beta\sin\beta\,\mathrm{Im}\lambda_5 + (1 + 2\sin^2\beta)\,\mathrm{Im}\lambda_7], \\ &a_{233} = \tfrac{1}{2}\{\sin\beta(\cos^2\beta\lambda_2 + \sin^2\beta\,\mathrm{Re}\lambda_{345} - 2\,\mathrm{Re}\lambda_5) + \cos\beta[\cos^2\beta\,\mathrm{Re}\lambda_7 + \sin^2\beta\,\mathrm{Re}(\lambda_6 - 2\lambda_7)]\}, \\ &a_{333} = \tfrac{1}{2}(\cos\beta\sin\beta\,\mathrm{Im}\lambda_5 - \sin^2\beta\,\mathrm{Im}\lambda_6 - \cos^2\beta\,\mathrm{Im}\lambda_7). \end{aligned} \tag{A4}$$

b. Quartic couplings

The quartic couplings involving two charged and two neutral Higgs fields are given by Eq. (A1), where:

$$\begin{aligned}
b_{11} &= \sin^2\beta\lambda_1 + \cos^2\beta\lambda_3 - 2\cos\beta\sin\beta\,\mathrm{Re}\lambda_6,\\
b_{12} &= -2[\cos\beta\sin\beta(\lambda_4 + \mathrm{Re}\lambda_5) - \sin^2\beta\,\mathrm{Re}\lambda_6\\
&\quad - \cos^2\beta\,\mathrm{Re}\lambda_7],\\
b_{13} &= 2\cos\beta[\cos\beta\sin\beta\,\mathrm{Im}\lambda_5 - \sin^2\beta\,\mathrm{Im}\lambda_6\\
&\quad - \cos^2\beta\,\mathrm{Im}\lambda_7],\\
b_{22} &= \cos^2\beta\lambda_2 + \sin^2\beta\lambda_3 - 2\cos\beta\sin\beta\,\mathrm{Re}\lambda_7,\\
b_{23} &= 2\sin\beta[\cos\beta\sin\beta\,\mathrm{Im}\lambda_5 - \sin^2\beta\,\mathrm{Im}\lambda_6\\
&\quad - \cos^2\beta\,\mathrm{Im}\lambda_7],\\
b_{33} &= \sin^4\beta\lambda_1 + \cos^4\beta\lambda_2 + 2\cos^2\beta\sin^2\beta\,\mathrm{Re}\lambda_{345}\\
&\quad - 4\cos\beta\sin\beta(\sin^2\beta\,\mathrm{Re}\lambda_6 + \cos^2\beta\,\mathrm{Re}\lambda_7).
\end{aligned} \tag{A5}$$

The quadrilinear couplings among four neutral Higgs fields are given by Eq. (A2), where:

$$\begin{aligned}
a_{1111} &= \tfrac{1}{8}\lambda_1, \qquad a_{1112} = \tfrac{1}{2}\mathrm{Re}\lambda_6,\\
a_{1113} &= -\tfrac{1}{2}\cos\beta\,\mathrm{Im}\lambda_6, \qquad a_{1122} = \tfrac{1}{4}\mathrm{Re}\lambda_{345},\\
a_{1123} &= -\tfrac{1}{2}(\cos\beta\,\mathrm{Im}\lambda_5 + \sin\beta\,\mathrm{Im}\lambda_6),\\
a_{1223} &= -\tfrac{1}{2}[\sin\beta\,\mathrm{Im}\lambda_5 + \cos\beta\,\mathrm{Im}\lambda_7],\\
a_{1133} &= \tfrac{1}{4}[\sin^2\beta\lambda_1 + \cos^2\beta(\lambda_3 + \lambda_4 - \mathrm{Re}\lambda_5)\\
&\quad - 2\cos\beta\sin\beta\,\mathrm{Re}\lambda_6],\\
a_{1222} &= \tfrac{1}{2}\mathrm{Re}\lambda_7, \qquad a_{2222} = \tfrac{1}{8}\lambda_2,\\
a_{2223} &= \tfrac{1}{2}\sin\beta\,\mathrm{Im}\lambda_7,\\
a_{1233} &= -\tfrac{1}{2}[-2\cos\beta\sin\beta\,\mathrm{Re}\lambda_5 + \sin^2\beta\,\mathrm{Re}\lambda_6\\
&\quad + \cos^2\mathrm{Im}\lambda_7],\\
a_{1333} &= \tfrac{1}{2}\cos\beta[\cos\beta\sin\beta\,\mathrm{Im}\lambda_5 - \sin^2\beta\lambda_6\\
&\quad - \cos^2\beta\,\mathrm{Im}\lambda_7],\\
a_{2233} &= \tfrac{1}{4}[\cos^2\beta\lambda_2 + \sin^2\beta(\lambda_3 + \lambda_4 - \mathrm{Re}\lambda_5)\\
&\quad - 2\cos\beta\sin\beta\,\mathrm{Re}\lambda_7],\\
a_{2333} &= \tfrac{1}{2}\sin\beta[\cos\beta\sin\beta\,\mathrm{Im}\lambda_5 - \sin^2\beta\,\mathrm{Im}\lambda_6\\
&\quad - \cos^2\mathrm{Im}\lambda_7],\\
a_{3333} &= \tfrac{1}{8}[\sin^4\beta\lambda_1 + \cos^4\beta\lambda_2 + 2\cos^2\beta\sin^2\beta\,\mathrm{Re}\lambda_{345}\\
&\quad - 4\sin\beta\cos\beta(\sin^2\beta\,\mathrm{Re}\lambda_6 + \cos^2\beta\,\mathrm{Re}\lambda_7)].
\end{aligned} \tag{A6}$$

2. The CP-conserving, soft Z_2-violating case

Below we collect couplings for the CP-conserving, explicitly soft Z_2-violating case, $\lambda_6 = \lambda_7 = \mathrm{Im}\lambda_5 = 0$.

a. Couplings in terms of λ_i, α, β

First, for completeness we present well-known couplings using our potential.

Trilinear couplings.—For the CP-even Higgs bosons we have

$$\begin{aligned}
g_{hhh} &= 3v[-\cos\beta\sin^3\alpha\lambda_1 + \sin\beta\cos^3\alpha\lambda_2\\
&\quad - \tfrac{1}{2}\sin2\alpha\cos(\beta+\alpha)\lambda_{345}],\\
g_{Hhh} &= v\{3\cos\beta\cos\alpha\sin^2\alpha\lambda_1 + 3\sin\beta\sin\alpha\cos^2\alpha\lambda_2\\
&\quad + [(1 - 3\sin^2\alpha)\cos(\beta+\alpha) - \sin\beta\sin\alpha]\lambda_{345}\},\\
g_{HHh} &= v\{-3\cos\beta\sin\alpha\cos^2\alpha\lambda_1 + 3\sin\beta\cos\alpha\sin^2\alpha\lambda_2\\
&\quad + [\cos\beta\sin\alpha + (1 - 3\sin^2\alpha)\sin(\beta+\alpha)]\lambda_{345}\},\\
g_{HHH} &= 3v[\cos\beta\cos^3\alpha\lambda_1 + \sin\beta\sin^3\alpha\lambda_2\\
&\quad + \tfrac{1}{2}\sin2\alpha\sin(\beta+\alpha)\lambda_{345}].
\end{aligned} \tag{A7}$$

For couplings involving the CP-odd A we have

$$\begin{aligned}
g_{AAA} &= g_{Ahh} = g_{AHH} = g_{AHh} = g_{AH^+H^-} = 0,\\
g_{AAh} &= v[-\cos\beta\sin^2\beta\sin\alpha\lambda_1 + \sin\beta\cos^2\beta\cos\alpha\lambda_2\\
&\quad + (\sin^3\beta\cos\alpha - \cos^3\beta\sin\alpha)\lambda_{345}\\
&\quad - 2\sin(\beta-\alpha)\lambda_5],\\
g_{AAH} &= v[\cos\beta\sin^2\beta\cos\alpha\lambda_1 + \sin\beta\cos^2\beta\sin\alpha\lambda_2\\
&\quad + (\cos^3\beta\cos\alpha + \sin^3\beta\sin\alpha)\lambda_{345}\\
&\quad - 2\cos(\beta-\alpha)\lambda_5].
\end{aligned} \tag{A8}$$

In the charged Higgs sector we have

$$\begin{aligned}
\frac{g_{hH^+H^-}}{v} &= \frac{\sin2\beta}{2}[\sin\beta\sin\alpha\lambda_1 - \cos\beta\cos\alpha\lambda_2\\
&\quad + \cos(\beta+\alpha)\lambda_{345}] - \sin(\beta-\alpha)\lambda_3,\\
\frac{g_{HH^+H^-}}{v} &= \frac{\sin2\beta}{2}[\sin\beta\cos\alpha\lambda_1 + \cos\beta\sin\alpha\lambda_2\\
&\quad - \sin(\beta+\alpha)\lambda_{345}] + \cos(\beta-\alpha)\lambda_3.
\end{aligned} \tag{A9}$$

Quartic couplings.—In the CP-even sector we have: $\frac{3}{2}$

$$\begin{aligned}
g_{hhhh} &= 3[\sin^4\alpha\lambda_1 + \cos^4\alpha\lambda_2 + \tfrac{1}{2}\sin^2 2\alpha\lambda_{345}],\\
g_{hhhH} &= \tfrac{3}{2}\sin2\alpha[-\sin^2\alpha\lambda_1 + \cos^2\alpha\lambda_2 - \cos2\alpha\lambda_{345}],\\
g_{hhHH} &= \tfrac{3}{4}\sin^2 2\alpha(\lambda_1 + \lambda_2) + (1 - \tfrac{3}{2}\sin^2 2\alpha)\lambda_{345},\\
g_{hHHH} &= \tfrac{3}{2}\sin2\alpha[-\cos^2\alpha\lambda_1 + \sin^2\alpha\lambda_2 + \cos2\alpha\lambda_{345}],\\
g_{HHHH} &= 3[\cos^4\alpha\lambda_1 + \sin^4\alpha\lambda_2 + \tfrac{1}{2}\sin^2 2\alpha\lambda_{345}].
\end{aligned} \tag{A10}$$

Quartic couplings involving the CP-odd A:

$$\begin{aligned}
g_{hhhA} &= g_{hhHA} = g_{hHHA} = g_{HHHA} = g_{hAAA} = g_{HAAA} = 0,\\
g_{hhAA} &= \sin^2\beta\sin^2\alpha\lambda_1 + \cos^2\beta\cos^2\alpha\lambda_2\\
&\quad + (\cos^2\beta\sin^2\alpha + \sin^2\beta\cos^2\alpha)\lambda_{345}\\
&\quad - \{1-\cos[2(\beta-\alpha)]\}\lambda_5,\\
g_{hHAA} &= \tfrac{1}{2}\sin2\alpha[-\sin^2\beta\lambda_1 + \cos^2\beta\lambda_2 - \cos2\beta\lambda_{345}]\\
&\quad - \sin[2(\beta-\alpha)]\lambda_5,\\
g_{HHAA} &= \sin^2\beta\cos^2\alpha\lambda_1 + \cos^2\beta\sin^2\alpha\lambda_2\\
&\quad + (\cos^2\beta\cos^2\alpha + \sin^2\beta\sin^2\alpha)\lambda_{345}\\
&\quad - \{1+\cos[2(\beta-\alpha)]\}\lambda_5,\\
g_{AAAA} &= 3[\sin^4\beta\lambda_1 + \cos^4\beta\lambda_2 + \tfrac{1}{2}\sin^2 2\beta\lambda_{345}]. \qquad \text{(A11)}
\end{aligned}$$

Quartic couplings involving the charged Higgs bosons:

$$\begin{aligned}
g_{hhH^+H^-} &= \sin^2\beta\sin^2\alpha\lambda_1 + \cos^2\beta\cos^2\alpha\lambda_2\\
&\quad + \tfrac{1}{2}\{1-\cos[2(\beta-\alpha)]\}\lambda_3\\
&\quad + \tfrac{1}{2}\sin2\beta\sin2\alpha\lambda_{345},\\
g_{hHH^+H^-} &= \tfrac{1}{2}\sin2\alpha(-\sin^2\beta\lambda_1 + \cos^2\beta\lambda_2)\\
&\quad + \tfrac{1}{2}\sin[2(\beta-\alpha)]\lambda_3 - \tfrac{1}{2}\sin2\beta\cos2\alpha\lambda_{345},\\
g_{HHH^+H^-} &= \sin^2\beta\cos^2\alpha\lambda_1 + \cos^2\beta\sin^2\alpha\lambda_2\\
&\quad + \tfrac{1}{2}\{1+\cos[2(\beta-\alpha)]\}\lambda_3\\
&\quad - \tfrac{1}{2}\sin2\beta\sin2\alpha\lambda_{345},\\
g_{hAH^+H^-} &= g_{HAH^+H^-} = 0,\\
g_{AAH^+H^-} &= \sin^4\beta\lambda_1 + \cos^4\beta\lambda_2 + \tfrac{1}{2}\sin^2 2\beta\lambda_{345},\\
g_{H^+H^-H^+H^-} &= 2[\sin^4\beta\lambda_1 + \cos^4\beta\lambda_2 + \tfrac{1}{2}\sin^2 2\beta\lambda_{345}]. \qquad \text{(A12)}
\end{aligned}$$

b. Trilinear couplings in terms of masses

It is useful to express parameters λ_i via Higgs boson masses and mixing angles with the aid of Eqs. (4.5) and (4.12). We get

$$\begin{aligned}
\lambda_1 &= \frac{1}{\cos^2\beta}\left[\frac{\cos^2\alpha M_H^2 + \sin^2\alpha M_h^2}{v^2} - \nu\sin^2\beta\right],\\
\lambda_2 &= \frac{1}{\sin^2\beta}\left[\frac{\sin^2\alpha M_H^2 + \cos^2\alpha M_h^2}{v^2} - \nu\cos^2\beta\right],\\
\lambda_{345} &= \frac{\sin2\alpha}{\sin2\beta}\frac{M_H^2 - M_h^2}{v^2} + \nu,\\
\lambda_4 &= \frac{M_A^2 - 2M_{H^\pm}^2}{v^2} + \nu,\\
\lambda_5 &= -\frac{M_A^2}{v^2} + \nu. \qquad \text{(A13)}
\end{aligned}$$

Now one can express triple Higgs couplings via masses β and α—this way a dependence on the parameter ν emerges.

For CP-even Higgs bosons

$$\begin{aligned}
g_{hhh} &= \frac{3}{v\sin2\beta}[(\cos\beta\cos^3\alpha - \sin\beta\sin^3\alpha)M_h^2\\
&\quad - \cos^2(\beta-\alpha)\cos(\beta+\alpha)\nu v^2],\\
g_{Hhh} &= \frac{1}{2v\sin2\beta}\cos(\beta-\alpha)[\sin2\alpha(2M_h^2 + M_H^2)\\
&\quad + (\sin2\beta - 3\sin2\alpha)\nu v^2],\\
g_{HHh} &= \frac{1}{2v\sin2\beta}\sin(\beta-\alpha)[-\sin2\alpha(M_h^2 + 2M_H^2)\\
&\quad + (\sin2\beta + 3\sin2\alpha)\nu v^2],\\
g_{HHH} &= \frac{3}{v\sin2\beta}[(\sin\beta\cos^3\alpha + \cos\beta\sin^3\alpha)M_H^2\\
&\quad - \sin^2(\beta-\alpha)\sin(\beta+\alpha)\nu v^2]. \qquad \text{(A14)}
\end{aligned}$$

For interactions with A

$$\begin{aligned}
g_{hAA} &= \frac{1}{v}\left[(2M_A^2 - M_h^2)\sin(\beta-\alpha)\right.\\
&\quad \left. + (M_h^2 - \nu v^2)\frac{\cos(\alpha+\beta)}{\sin\beta\cos\beta}\right],\\
g_{HAA} &= \frac{1}{v}\left[(2M_A^2 - M_H^2)\cos(\beta-\alpha) + (M_H^2 - \nu v^2)\right.\\
&\quad \left. \times\frac{\cos(\alpha+\beta)}{\sin\beta\cos\beta}\right]. \qquad \text{(A15)}
\end{aligned}$$

For interactions with $H^\pm$

$$\begin{aligned}
g_{hH^+H^-} &= \frac{1}{v}\left[(2M_{H^\pm}^2 - M_h^2)\sin(\beta-\alpha)\right.\\
&\quad \left. + \frac{(M_h^2 - \nu v^2)\cos(\beta+\alpha)}{\sin\beta\cos\beta}\right]\\
&= \frac{1}{v}\left[(2M_{H^\pm}^2 + M_h^2 - 2\nu v^2)\sin(\beta-\alpha)\right.\\
&\quad \left. + 2(M_h^2 - \nu v^2)\cos(\beta-\alpha)\cot2\beta\right],\\
g_{HH^+H^-} &= \frac{1}{v}\left[(2M_{H^\pm}^2 - M_H^2)\cos(\beta-\alpha)\right.\\
&\quad \left. + \frac{(M_H^2 - \nu v^2)\sin(\beta+\alpha)}{\sin\beta\cos\beta}\right]\\
&= \frac{1}{v}[(2M_{H^\pm}^2 + M_H^2 - 2\nu v^2)\cos(\beta-\alpha)\\
&\quad - 2(M_H^2 - \nu v^2)\sin(\beta-\alpha)\cot2\beta]. \qquad \text{(A16)}
\end{aligned}$$

c. Trilinear couplings in terms of masses and relative couplings in model II

For the model II for the interaction with fermions we find (denoting by ϕ either h or H)

$$\begin{aligned}
g_{\phi\phi\phi} &= \frac{3}{2v}[(\chi_u^\phi + \chi_d^\phi - \chi_V^\phi \chi_u^\phi \chi_d^\phi)(M_\phi^2 - \nu v^2) + \chi_V^\phi \nu v^2],\\
g_{\phi_1\phi_2\phi_2} &= -\frac{1}{2v}\chi_V^{\phi_1}[\chi_u^{\phi_2}\chi_d^{\phi_2}(2M_{\phi_2}^2 + M_{\phi_1}^2 - 3\nu v^2) - \nu v^2] \quad (\phi_1 \neq \phi_2),\\
g_{\phi AA} &= \frac{1}{v}[(2M_A^2 - M_\phi^2)\chi_V^\phi + (M_\phi^2 - \nu v^2)(\chi_u^\phi + \chi_d^\phi)],\\
g_{A\phi_1\phi_2} &= g_{AAA} = g_{AH^+H^-} = 0,\\
g_{\phi H^+H^-} &= \frac{1}{v}[(2M_{H^\pm}^2 - M_\phi^2)\chi_V^\phi + (M_\phi^2 - \nu v^2)(\chi_u^\phi + \chi_d^\phi)].
\end{aligned} \tag{A17}$$

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