Symmetries in Two Higgs Doublet Model, CP violation and heavy Higgs effects

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We apply the invariance of physical picture under a change of Lagrangian – the reparametrization invariance in the space of Lagrangians and its particular case – the rephrasing invariance – for analysis of the Two Higgs Doublet Model. We found that some parameters of theory like $\tan\beta$ are reparametrization dependent and therefore cannot be fundamental. We use the Z_2-symmetry of the Lagrangian, which prevents a $\phi_1 \leftrightarrow \phi_2$ transitions, and the different levels of its violation to describe a physical content of the model. In general a theory with broken Z_2-symmetry describes a CP violation in the physical Higgs sector. We argue that the 2HDM with a soft breaking of Z_2-symmetry is a natural model in the description of EWSB.

We determine the range of parameters for which CP violation and Flavor Changing Neutral Current effects are naturally small, what corresponds to a small dimensionless mass parameter $\nu = \mathrm{Re}\, m_{12}^2/(2v_1v_2)$ (in the real vacuum form of Lagrangian – without phase difference among vacuum expectation values of ϕ_1 and ϕ_2). We discuss how for small ν some Higgs bosons can be heavy, with mass up to about 0.6 TeV, without violation of the unitarity constraints. All physical Higgs bosons, except one, can be arbitrary heavy if ν is large. We analyse main features of this case, which for $\nu \to \infty$ corresponds 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 to analyse different physical situations (including CP violation) in terms of these couplings, instead of parameters of Lagrangian.

I. INTRODUCTION

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

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

Here, $\mathcal{L}_{gf}^{SM}$ 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) the single scalar isodoublet with hypercharge $Y=1$ is implemented. Here $\mathcal{L}_H = (D_\mu\phi)^\dagger D_\mu\phi - V$, with the Higgs potential $V = \lambda\phi^4/2 - m^2\phi^2/2$, its minimum describes the vacuum expectation value v as $\langle\phi\rangle = v/\sqrt{2} = \sqrt{m^2/2\lambda}$. In the SM, the couplings of the physical Higgs boson to gauge bosons can be expressed via masses as $g_W^{\rm SM} = \sqrt{2}M_W/v$, $g_Z^{\rm SM} = \sqrt{2}M_Z/v$, and Yukawa term has a form:

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

Below we consider the simplest extension of the SM, the Two Higgs Doublet Model (2HDM) ([1], see e.g. [2] for definitions). We treat a CP violation in the Higgs sector as a natural feature of theory.

• Sec. II A: The 2HDM 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 phases. Each this transformation generates new Lagrangian, with parameters, given by those of incident Lagrangian and parameters of transformation (*the reparametrization transformation*). Therefore, the physical reality described by some Lagrangian $\mathcal{L}$ (*physical model*) is also described by many other Lagrangians. We call this property by the *reparametrization invariance in a space of Lagrangians (with coordinates given by its parameters).* In other words, the Lagrangian describes unambiguously some physical reality as in usual case, however, given physical reality can be described by a different (reparametrization equivalent) Lagrangians. We discuss also a particular case of the reparametrization invariance – *a rephasing invariance.*

• Sec. II B: One of the earliest reason for introducing the 2HDM was to describe the phenomenon of CP violation [3], an effect which can be potentially large. Glashow and Weinberg [4] realized that the CP violation and the flavour changing neutral currents (FCNC) can be naturally suppressed by imposing in Lagrangian a Z_2 symmetry, that is the invariance on the Lagrangian under the interchange

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

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 (FCNC) effects. The Yukawa interaction can lead (via loop corrections) to the CP-violation even if CP violation is absent in the basic Higgs Lagrangian. Imposing specific constraints on $\mathcal{L}_Y$ allows to eliminate this source of 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.

• Sec. II C: The EWSB is described by nonzero vacuum expectation values of fields $\phi_{1,2}$ with generally different phases. This phase difference can be eliminated by a suitable rephasing transformation, resulting *a real vacuum form of Lagrangian*, we use this form of Lagrangian in the main part of paper. Here real and imaginary parts of 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 (in addition to v.e.v.'s and quartic coefficients of Lagrangian), while the imaginary part (describing CP violation) is given by these v.e.v.'s and quartic coefficients of Lagrangian.

• Sec. III: Next we come from ϕ_i to the observable (physical) Higgs particles. The Goldstone modes and charged $H^{\pm}$ 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 definite CP parity. The interaction of matter with these states gives observable effects of CP violation. The analyses of CP violation effects become very transparent if a two–step procedure of diagonalization is used, with the first step corresponding to the diagonalization of η_1, η_2 states. This leads to the states h and H, discussed usually in context of the CP–conserving case. It allows us to consider the general CP nonconserving case (second step) in terms of states h, H and A, customary in the case of CP conservation.

• Sect. IV: A most general form of Yukawa interaction violates CP symmetry, gives 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 proper Higgs Lagrangian $\mathcal{L}_H$. With such Yukawa sector the CP violation is obliged only by a structure of the Higgs Lagrangian, and FCNC effects can be naturally small. Here we consider the well known Model II [2] in the explicit form, which is defined with accuracy up to rephasing transformation.

In the subsequent discussion it is useful to define 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 ($j = W, Z, u, d, \ell...$), to the corresponding SM couplings – *relative couplings*:

$$\chi_j^{(i)} = g_j^{(i)}/g_j^{\rm SM}\,, \qquad (1.3)$$

As their squared values are in principle measurable, we treat $\chi_j^{(i)}$ themselves as measurable quantities.

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

• Sec. V: Parameters of Lagrangian are constrained by positivity (vacuum stability) and minimum constraints. 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. This should be reliable for not too large values of parameters of the Lagrangian; we study the relevant *unitarity and perturbativity constraints*. Most of above constraints were obtained in literature in the case of soft violation of Z_2 symmetry. We discuss main new aspects in the case of hard violation of Z_2 symmetry in sec. V C.

• Sec. VI: In 2HDM there is an attractive possibility that one of neutral Higgs bosons h_1 is similar to that in the SM while others are much heavier. The studies of 2HDM are based often on an assumption of *decoupling* of these heavy Higgs bosons from known particles, i.e. effects of these additional Higgs bosons disappear if their masses tend to infinity. This specific property is an natural one in *constructing* of a new theory at extremely large energies (small distances), since it provides a self-consistent description of phenomena in our world. However, it is not necessary for the description of phenomena in the presence of heavy but not extremely heavy new particles. In the used real vacuum form of the Lagrangian the mentioned phenomenon is governed by a singe dimensionless parameter $\nu \propto \,{\rm Re}\, m_{12}^2$. For large ν the decoupling limit is realized, i.e. the mentioned above 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 analyse properties of all Higgs bosons and their interactions in this decoupling limit. At small ν, the masses of such additional Higgs bosons are bounded from above by the unitarity constraints. These additional 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, respecting the unitarity constraints. We argue that this non–decoupling option of 2HDM is more *natural* for weak CP violation and FCNC (in spirit of t'Hooft's concept of naturalness [5]).

II. HIGGS LAGRANGIAN

To keep the value $\rho = M_W^2/(M_Z^2\cos^2\theta_W)$ 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 of doublets (the other choice, $Y_1=1$, $Y_2=-1$, is used in the MSSM; this case is also described by equations below with a trivial change of variables).

The most general renormalizable Higgs Lagrangian for the fields $\phi_{1,2}$ 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, V is the Higgs potential:

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

$$\begin{aligned} V = \frac{\lambda_1}{2}(\phi_1^\dagger\phi_1)^2 + \frac{\lambda_2}{2}(\phi_2^\dagger\phi_2)^2\\ +\lambda_3(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_4(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1)\\ +\frac{1}{2}\left[\lambda_5(\phi_1^\dagger\phi_2)^2 + \text{h.c.}\right]\\ +\left\{\left[\lambda_6(\phi_1^\dagger\phi_1) + \lambda_7(\phi_2^\dagger\phi_2)\right](\phi_1^\dagger\phi_2) + \text{h.c.}\right\} \end{aligned} \tag{2.1c}$$

$$\begin{aligned} -\frac{1}{2}\left\{m_{11}^2(\phi_1^\dagger\phi_1) + m_{22}^2(\phi_2^\dagger\phi_2)\right.\\ \left.+\left[m_{12}^2(\phi_1^\dagger\phi_2) + \text{h.c.}\right]\right\}. \end{aligned} \tag{2.1d}$$

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. Therefore, this potential contains 14 independent parameters and the entire Higgs Lagrangian – 16. We will see that CP violation in Higgs sector, which is a very natural feature of 2HDM, can appear only if some of these coefficients are not real.

A. Reparametrization and rephasing invariance

1. Reparametrization invariance

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

$$\begin{pmatrix}\phi'_1\\ \phi'_2\end{pmatrix} = \hat{\mathcal{F}}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}\,, \tag{2.2}$$

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

• **In the $\varkappa=0$ case** the transformation (2.2) does not change the form of kinetic term but induces the changes of coefficients of Lagrangian $\lambda_i\to\lambda'_i$, $m_{ij}^2\to(m')_{ij}^2$ which we call **reparametrization transformation** with

$$\begin{aligned} &\lambda'_1 = c^2\lambda_1 + s^2\lambda_2 - cs\Phi - 2cs\,\mathrm{Re}\,(\tilde\lambda_6+\tilde\lambda_7),\\ &\lambda'_2 = s^2\lambda_1 + c^2\lambda_2 - cs\Phi + 2cs\,\mathrm{Re}\,(\tilde\lambda_6+\tilde\lambda_7),\\ &\lambda'_3 = \lambda_3 + cs\Phi,\quad \lambda'_4 = \lambda_4 + cs\Phi,\\ &e^{2i\rho}\lambda'_5 = \lambda_5 +\\ &e^{i\tau}\left[cs\Phi + 2is^2\,\mathrm{Im}\,\tilde\lambda_5 - 2ics\,\mathrm{Im}\,(\tilde\lambda_6-\tilde\lambda_7)\right],\\ &e^{i\rho}\lambda'_6 = c^2\lambda_6 - s^2\lambda_7 + \frac{e^{i\tau}}{2}cs(\lambda_1-\lambda_2+\Psi),\\ &e^{i\rho}\lambda'_7 = c^2\lambda_7 - s^2\lambda_6 + \frac{e^{i\tau}}{2}cs(\lambda_1-\lambda_2-\Psi),\\ &(m')_{11}^2 = c^2m_{11}^2 + s^2m_{22}^2 - 2cs\mu_{12}^2,\\ &(m')_{22}^2 = s^2m_{11}^2 + c^2m_{22}^2 + 2cs\mu_{12}^2,\\ &e^{i\rho}(m')_{12}^2 = m_{12}^2 +\\ &e^{i\tau}\left[cs(m_{11}^2-m_{22}^2) - 2s^2\mu_{12}^2\right]. \end{aligned} \tag{2.3}$$

where $c=\cos\theta$, $s=\sin\theta$, $\mu_{12}^2 = \mathrm{Re}\,(m_{12}^2e^{-i\tau})$, $\tilde\lambda_5 = \lambda_5e^{-2i\tau}$, $\tilde\lambda_{6,7} = \lambda_{6,7}e^{-i\tau}$ and

$$\Phi_0 = \lambda_1+\lambda_2 - 2(\lambda_3+\lambda_4+\,\mathrm{Re}\,\tilde\lambda_5),$$

$$\Phi = cs\Phi_0 + 2(c^2-s^2)\,\mathrm{Re}\,(\tilde\lambda_6-\tilde\lambda_7),$$

$$\Psi = (c^2-s^2)\Phi_0 - 8cs\,\mathrm{Re}\,(\tilde\lambda_6-\tilde\lambda_7) + 2i\,\mathrm{Im}\,\tilde\lambda_5.$$

By construction, the Lagrangians of the form (2.1) with coefficients λ_i, m_{ij}^2 and that with coefficients λ'_i, $(m')_{ij}^2$ (2.3) describe the same physical reality. We call this property a **reparametrization invariance**.

The set of *reparametrization transformations* (2.3) represents the 3–parametrical **reparametrization transformation group 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_{ii}^2, $\mathrm{Re}\,(m_{12}^2)$, $\mathrm{Im}\,(m_{12}^2)$, $\mathrm{Re}\,\varkappa$, $\mathrm{Im}\,\varkappa$ with *reparametrization parameters* ρ, θ, τ (similar to the gauge parameter of gauge theories). The transformations $\hat{\mathcal{F}}$ (2.2) represent this very group in the space of fields ϕ_i (*the scalar basis*). It contains in addition free parameter ρ_0, which describes **an overall phase freedom**.

A set of physically equivalent Higgs Lagrangians, obtained from each other by transformations (2.3) forms *the reparametrization equivalent space*, which is 3-dimensional subspace of the entire space of Lagrangians. The parameters of Lagrangian can be determined in principle only with accuracy up to the reparametrization freedom, the different Lagrangians within *the reparametrization equivalent space* are physically equivalent.

Among the reparametrization equivalent Lagrangians one can distinguish such, which possess some defined property in an explicit form. They occupy some domain in the reparameterization equivalent space. We call such set of Lagrangians "a family", adding in front words describing property of model which are explicit for all Lagrangians of this family (fig. 1) and use for particular Lagrangian of this family word "a form".

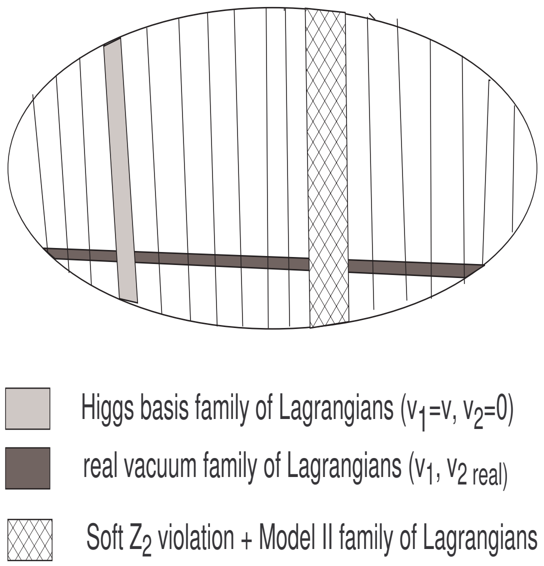

FIG. 1: *Schematic presentation of reparametrization equivalent space of Lagrangians. Different strips represent families with different explicit properties. A particular case where the soft Z_2 violating and Model II Lagrangians families coincide is shown.*

• **In the $\varkappa \neq 0$ case** the reparametrization transformation (2.2) induces in addition transformation 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

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

So, in order to restore a canonical form of kinetic term a field renormalization is needed in addition to the transformations (2.3). This case will be discussed in more detail elsewhere [7].

Remark on physical parameters.

Some parameters of theory which are treated often as physical (and in principle measurable) are in fact reparametrization dependent. The most important example provides a ratio of vacuum expectation values of scalar fields, $\tan\beta$ (2.11). For example, under the transformation (2.2) with $\rho = \xi$ (see eq. (2.11b)) and $\tau = 0$, angle β changes to $\beta + \theta$.

2. Rephasing invariance

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

$$\begin{gathered} \phi_i \to e^{-i\rho_i}\phi_i, \quad (i = 1, 2), \\ \rho_1 = \rho_0 - \frac{\rho}{2},\;\; \rho_2 = \rho_0 + \frac{\rho}{2},\;\; \rho = \rho_2 - \rho_1. \end{gathered} \tag{2.5}$$

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

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

By construction, the Lagrangians of form (2.1) with coefficients λ_i, m_{ij}^2 and with coefficients given by eq. (2.6) describe the same physical reality. We call this property the **rephasing invariance**, which is similar to the definition given in [12].

The transformations (2.6) represent the 1–parametrical **rephasing transformation group** with parameter ρ, called by us *the rephasing parameter*. By construction, this group is a subgroup of the reparametrization group. The transformations (2.5) represent the rephasing transformation group in the space of fields ϕ_i.

The 1-dimensional *rephasing equivalent space*, being a subspace of the entire (3-dimensional) reparametrization equivalent space of Lagrangians, is given by the sets of parameters of Lagrangians at different ρ. One can say that the entire reparametrization equivalent space is sliced to the rephasing equivalent subspaces (strips in fig. 1).

Two remarks.

• The concept of rephasing invariance is easily extended to the description of a whole system of scalars and fermions (4.2). The reparametrization transformations for scalar fields (2.2) evidently induce changes into the set of Yukawa couplings. This may hide some properties of Yukawa Lagrangian, which are explicit in a definite scalar basis (e.g. Model I or Model II, see sec. IV). The Kobyashi – Maskawa matrix represent the reparameterization transformation from the QCD to electroweak basis for fermions.

• We will see later that CP symmetry is conserved in the Higgs sector if all parameters of Lagrangian (2.1) are real. Obviously, the CP–violation does not appear if the Lagrangian with complex parameters can be transformed to a form with all real parameters by means of some reparametrization (2.2).

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 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 the Z_2 symmetry*, and of the operator dimension 4 (with $\lambda_{6,7}$ and $\varkappa$), called *a hard violation of the Z_2 symmetry.*

a. An exact $\boldsymbol{Z_2}$ *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 rephasing transformation (2.6) with a suitable phase ρ allows to get another (rephasing equivalent) form of Lagrangian with a real λ_5.

b. A soft violation of $\boldsymbol{Z_2}$ *symmetry.* In the case of soft violation of Z_2 symmetry one adds to the Z_2 symmetric Lagrangian the term $m_{12}^2(\phi_1^\dagger\phi_2) + h.c.$, 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 different rephasing transformations (2.6) applied to the Lagrangian with a softly broken Z_2 symmetry can not 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 broken Z_2 symmetry. These new terms break Z_2 symmetry *at both large and small distances* – this is called a hard violation of Z_2 symmetry. We discuss here the case of the *true hard violation of Z_2 symmetry*, which cannot be transformed to the case of Z_2 conservation, nor its soft violation, by any reparametrization transformation (2.3).

C. The case of hidden soft Z_2 violation

Let us assume that there exists some ϕ_1, ϕ_2 basis, in which our physical model is described by the Lagrangian with exact or softly violated Z_2 symmetry, $\mathcal{L}_s$. The general reparametrzation transformation (2.3) converts this Lagrangian to a form $\mathcal{L}_{hs}$ with λ_6, $\lambda_7 \neq 0$ and $\varkappa = 0$, which looks like the Lagrangian with hard Z_2 violation. 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 rephasing transformation (2.6), eliminating the phase of λ_5 and obtain the Lagrangian $\mathcal{L}_s^R$ with real λ_5 (in this case m_{12}^2 can be complex leaving open an opportunity for CP violation). Then we apply to $\mathcal{L}_s^R$ a general reparameterization transformation (2.3) and obtain Lagrangian in the form (2.1) with generally complex λ_5 and nonzero $\lambda_{6,7}$ (but still $\varkappa = 0$). In this case the equations (2.3) simplify, we get new quartic couplings in a form

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

The eq-s (2.7) allow to find parameters of the mentioned Lagrangian $\mathcal{L}_s^R$. To this goal it is useful to consider following consequence of combinations of eq-s (2.7):

$$\begin{aligned}
&\frac{\lambda_6' + \lambda_7'}{\lambda_6'^* + \lambda_7'^*} = e^{2i(\tau-\rho)}\,,\\
&\frac{\lambda_6' + \lambda_7'}{\lambda_1' - \lambda_2'} = e^{i(\tau-\rho)}\frac{\tan 2\theta}{2}\,,\\
&e^{-i\rho}\lambda_5 = \lambda_5' - e^{2i(\tau-\rho)}[cs\Phi + +2is^2\sin 2\tau\lambda_5].\\
&e^{-i(\tau-\rho)}(\lambda_6' - \lambda_7') = (c^2 - s^2)\Phi + 2ics\lambda_5\sin 2\tau.
\end{aligned} \tag{2.8}$$

(1) The value of $\tau - \rho$ is determined from the first equation. (2) After that one can determine angle θ via second equation. (3) Next one can determine quantity Φ and $2cs\lambda_5\sin 2\tau$ as the real and imaginary parts of the form in the fourth line. (4) After that one can determine the angle ρ and the parameter λ_5 via the phase and the module of the quantity in third line. (5) Now all remaining quantities λ_{1-4} can be determined easily from the first four equations (2.7).

Equations in the third and fourth lines represent two different ways of obtaining the parameter λ_5. Besides, quantity Φ can be obtained both via these equations and from 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 for the Lagrangian. It shows explicitly that in this case the quartic sector is described by only 8 independent parameters (λ_{1-5} and θ, ρ, τ) instead of 10 independent parameters of the general Lagrangian (2.1) (λ_{1-4}, $\mathrm{Re}\,\lambda_{5-7}$, $\mathrm{Im}\,\lambda_{5-7}$).

D. Some features of true hard Z_2 violation

Let us discuss briefly what should be done in the case of hard violation of Z_2 symmetry with the mixed kinetic terms, i.e. $\varkappa \neq 0$ in Eq. (2.1b). These kinetic terms 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, non-diagonal two-point functions leads anyway to the mixed kinetic terms (e.g. from $\lambda_6^*\lambda_{1,3-5}$ and $\lambda_7^*\lambda_{2-5}$ loops). It means that $\varkappa$ becomes nonzero at the higher orders of perturbation theory, and *vice versa* a mixed kinetic term generates counter-terms 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 [8, 9]). (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 [10].) Note that the parameter $\varkappa$ is generally running like parameters λ's. Therefore, the Lagrangian *remains off–diagonal* in fields ϕ_i even at very small distances, above the EWSB transition. Such theory seems to be *unnatural*.

To find the signature of this case in the arbitrary form of Lagrangian, it is useful to consider polarization operator matrix $\mathcal{P} = \begin{pmatrix} \Pi_{11} & \Pi_{12} \\ \Pi_{21} & \Pi_{22} \end{pmatrix}$. In the general case the ratio $\Pi_{12}/(\Pi_{11} - \Pi_{22})$ is running quantity at large Higgs boson virtuality k^2 in contrast with the case of 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 sect II C. The one–loop polarization operator for two fields has a form $\mathcal{P} = \begin{pmatrix} \Pi_1^s & 0 \\ 0 & \Pi_2^s \end{pmatrix} k^2 + \textit{finite terms}$, for $k^2 \to \infty$. The terms Π_1^s, 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 reparametrization transformation (2.2), 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 gives the nonzero mixed polarization operator:

$$\mathcal{P}' = \begin{pmatrix} \Pi_{11} & \Pi_{12} \\ \Pi_{12}^* & \Pi_{22} \end{pmatrix} k^2 + \textit{finite terms},$$
$$\Pi_{11} = \Pi_1^s \cos^2\theta + \Pi_2^s \sin^2\theta,$$
$$\Pi_{12} = (\Pi_1^s - \Pi_2^s) e^{-i\tau} \sin\theta\cos\theta,$$
$$\Pi_{22} = \Pi_2^s \cos^2\theta + \Pi_1^s \sin^2\theta.$$

Naively, this form of polarization operator suggests that one should introduce in Lagrangian the mixed kinetic term $\propto (D_\mu\phi_1)^\dagger D_\mu\phi_2 + h.c.$ However, inverse reparametrization transformation restores the incident form of $\mathcal{L}_H$ with soft Z_2 symmetry violation, i.e. without kinetic terms, i.e. without $\phi_1 \leftrightarrow \phi_2$ transitions at small distances. Therefore, the mentioned relations among parameters of new quartic terms prevent an appearance of the mixed kinetic term in Higgs Lagrangian in any reparametrization equivalent form of Lagrangian. The renormalization group analysis ensures that for the Lagrangian $\mathcal{L}_{hs}$ the ratio $\Pi_{12}/(\Pi_{11} - \Pi_{22})$ at large k^2 is renormalization invariant quantity, i.e. it is independent on normalization scale Λ. 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 reparameterization transformation (2.3) and the ratio $\Pi_{12}/(\Pi_{11} - \Pi_{22})$ at large k^2 is renormalization invariant the ratio $\Pi_{12}/(\Pi_{11} - \Pi_{22})$ at large k^2 is renormalization dependent quantity.

Besides, it is instructive to consider in more detail the case of soft violation of Z_2 symmetry. The EWSB procedure (sec. II E) transforms the Lagrangian expressed in terms of fields ϕ_i to that written in terms of Higgs fields h_{1-3} and $H^\pm$. In this form 18 quartic couplings appear but there are some relations among them, since all of them are obtained from the initial Lagrangian $\mathcal{L}_s$ with 6 parameters (λ_{1-4}, $\mathrm{Re}\,\lambda_5$, $\mathrm{Im}\,\lambda_5$) and the orthogonal transformation from the (ϕ_1, ϕ_2) basis to ($H^\pm$, h_1, h_2, h_3) basis with the additional 3 parameters. In this Lagrangian a mixed polarization operator may also appear, however no mixed kinetic term. This is due the mentioned relations among parameters of new quartic terms which prevent appearance of the mixed kinetic term in Higgs Lagrangian [11]. 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. IV.

The diagonalization (2.9) is rather special and it may change even the definitions of λ's, what would destroy relatively simple relations between the masses of the Higgs bosons (discussed below).

Although in this paper we present relations for a 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.

E. Vacuum. Used form of the potential

The minimum of the potential defines the vacuum expectation values (v.e.v) of the fields ϕ_i:

$$\left.\frac{\partial V}{\partial \phi_1}\right|_{\substack{\phi_1=\langle\phi_1\rangle,\\ \phi_2=\langle\phi_2\rangle}} = 0, \qquad \left.\frac{\partial V}{\partial \phi_2}\right|_{\substack{\phi_1=\langle\phi_1\rangle,\\ \phi_2=\langle\phi_2\rangle}} = 0. \tag{2.10}$$

In order to describe the $U(1)$ symmetry of electromagnetism and using the overall phase freedom of the Lagrangian to choose one vacuum expectation value real [12, 13] we take:

$$\langle\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v_1\end{pmatrix} \quad\text{and}\quad \langle\phi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ v_2 e^{i\xi}\end{pmatrix}, \qquad (2.11a)$$

with a relative phase ξ. These v_i (and therefore parameters of whole Lagrangian) obey SM constraint: $v_1^2 + v_2^2 = v^2$, with $v = (\sqrt{2}G_{\rm F})^{-1/2} = 246$ GeV. The another parameterization of these v.e.v.'s (via parameters v and β) is also used:

$$v_1 = v\cos\beta,\quad v_2 = v\sin\beta,\qquad \beta\in(0,\,\pi/2)\,. \qquad (2.11b)$$

The rephasing transformation (2.5) shifts phase difference ξ as follows

$$\xi \to \xi - \rho\,. \qquad (2.12)$$

Therefore, the phase difference ξ between the v.e.v.'s has no physical sense (see e.g. [12]).

Let us take some Lagrangian describing our model and calculate v.e.v.'s (2.11). Than, by making rephasing transformation (2.6) with $\rho = \xi$, we get *the real vacuum form of Lagrangian* in which the relative phase of v.e.v.'s equals to zero. In accordance with eq. (2.6) we get

$$\begin{aligned}&\lambda_{1-4,rv} = \lambda_{1-4},\ \ \lambda_{5,rv} = \lambda_5 e^{-2i\xi},\\ &\lambda_{6,rv} = \lambda_6 e^{-i\xi},\ \ \lambda_{7,rv} = \lambda_7 e^{-i\xi},\\ &\varkappa_{rv} = \varkappa e^{-i\xi},\ \ m_{12,rv}^2 = m_{12}^2 e^{-i\xi}.\end{aligned} \qquad (2.13)$$

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:

$$\begin{aligned}\lambda_{345} &= \lambda_{3,rv} + \lambda_{4,rv} + \mathrm{Re}\,\lambda_{5,rv},\\ \lambda_{67} &= \frac{1}{2}\left(\frac{v_1}{v_2}\lambda_{6,rv} + \frac{v_2}{v_1}\lambda_{7,rv}\right),\\ \tilde\lambda_{67} &= \frac{1}{2}\left(\frac{v_1}{v_2}\lambda_{6,rv} - \frac{v_2}{v_1}\lambda_{7,rv}\right),\\ m_{12,rv}^2 &= 2v_1v_2(\nu + i\delta).\end{aligned} \qquad (2.14)$$

The minimum condition (2.10) does not constrain real part of $m_{12,rv}^2$, while this condition expresses the imaginary part of $m_{12,rv}$ via $\mathrm{Im}\,(\lambda_{5-7,rv})$:

$$\delta = \frac{1}{2}\,\mathrm{Im}\,\{\underbrace{\lambda_{5,rv}}_{soft} + \underbrace{2\lambda_{67}}_{hard}\}\,. \qquad (2.15)$$

Here (and in the subsequent equation) the first and second underbraced term are added to each other in the case of soft and hard violation of Z_2 symmetry, respectively (the latter term also appear in the case of hidden soft Z_2 violation). 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 are presented for the real vacuum form of potential, without explicit subscript rv. We will specially comment when other forms of Lagrangian will be discussed.

It is useful for subsequent calculations to change description of potential, containing three independent parameters m_{ij}^2, to the description with three other parameters related to the minimum: v_1, v_2 and ν. The eq-s (2.10), (2.10) allow to obtain

$$\begin{aligned}m_{11}^2 &= \underbrace{\lambda_1 v_1^2 + \lambda_{345}v_2^2}_{Z_2\ sym}\ \underbrace{-2\nu v_2^2}_{soft}\ + \underbrace{\frac{v_2}{v_1}\,\mathrm{Re}\,\left(3v_1^2\lambda_6 + v_2^2\lambda_7\right)}_{hard},\\ m_{22}^2 &= \underbrace{\lambda_2 v_2^2 + \lambda_{345}v_1^2}_{Z_2\ sym}\ \underbrace{-2\nu v_1^2}_{soft} + \underbrace{\frac{v_1}{v_2}\,\mathrm{Re}\,\left(v_1^2\lambda_6 + 3v_2^2\lambda_7\right)}_{hard}.\end{aligned} \qquad (2.16)$$

Using these relations we obtain other form of real vacuum potential, used in this paper:

$$\begin{aligned}V = &\frac{\lambda_1}{2}\left[(\phi_1^\dagger\phi_1) - \frac{v_1^2}{2}\right]^2 + \frac{\lambda_2}{2}\left[(\phi_2^\dagger\phi_2) - \frac{v_2^2}{2}\right]^2\\ &+\lambda_3(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_4(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1)\\ &+\frac{1}{2}\left[\lambda_5(\phi_1^\dagger\phi_2)^2 + \mathrm{h.c.}\right]\\ &+\left\{\left[\lambda_6(\phi_1^\dagger\phi_1) + \lambda_7(\phi_2^\dagger\phi_2)\right](\phi_1^\dagger\phi_2) + \mathrm{h.c.}\right\}\\ &-\frac{1}{2}\left(\lambda_{345} + 2\,\mathrm{Re}\,\lambda_{67}\right)[v_2^2(\phi_1^\dagger\phi_1) + v_1^2(\phi_2^\dagger\phi_2)]\\ &-\mathrm{Re}\,[\lambda_6(\phi_1^\dagger\phi_1) + \lambda_7(\phi_2^\dagger\phi_2)]v_1v_2\\ &+\nu(v_2\phi_1 - v_1\phi_2)^\dagger(v_2\phi_1 - v_1\phi_2)\\ &+2\delta\ \mathrm{Im}\,(\phi_1^\dagger\phi_2)v_1v_2.\end{aligned} \qquad (2.17)$$

In this form the quartic terms are as those in the initial potential (2.1) but with particular values λ_i equal to $\lambda_{i,rv}$. The mass term is determined via v.e.v.'s v_1, v_2 and the couplings λ_i plus a single *free* dimensionless parameter ν. The quantity $\delta \propto \mathrm{Im}\ m_{12}^2$ is constrained in this form by eq. (2.15).

In the above equation the soft Z_2 violating contribution is given by a sum of last two terms of (2.17), so that the variation of each of them don't influence v.e.v.'s. This decomposition is less transparent in Lagrangians with $\xi \neq 0$.

Remarks.

- The Higgs potential has also a minimum, violating a charge conservation ("charged vacuum"). At $\nu > 0$ the vacuum energy of this charged vacuum is higher than that for the neutral vacuum (2.10), see [13], [14]. That is why we discuss only minimum (2.10).
- The set of real vacuum Lagrangians (*real vacuum Lagrangian family*) forms a subspace in the entire reparametrization equivalent space, which is pictured in fig. 1 by black horizontal line. In different points of this subspace the $\tan\beta$ values are different.

III. PHYSICAL HIGGS SECTOR

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

A standard decomposition of the fields ϕ_i in terms of physical fields is made via

$$\phi_1 = \begin{pmatrix} \varphi_1^+ \\ \dfrac{v_1+\eta_1+i\chi_1}{\sqrt{2}} \end{pmatrix}, \quad \phi_2 = \begin{pmatrix} \varphi_2^+ \\ \dfrac{v_2+\eta_2+i\chi_2}{\sqrt{2}} \end{pmatrix}. \tag{3.1}$$

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, $G^0 = \cos\beta\,\chi_1 + \sin\beta\,\chi_2$, $G^\pm = \cos\beta\,\varphi_1^\pm + \sin\beta\,\varphi_2^\pm$, and the charged Higgs boson fields $H^\pm$,

$$H^\pm = -\sin\beta\,\varphi_1^\pm + \cos\beta\,\varphi_2^\pm\,, \tag{3.2}$$

with the mass squared equal to

$$M_{H^\pm}^2 = \left[\nu - \frac{1}{2}(\lambda_4 + \operatorname{Re}\lambda_5 + 2\operatorname{Re}\lambda_{67})\right]v^2. \tag{3.3}$$

- The reparametrization transformation (2.2) with $\tau = 0$, $\theta = -\beta$ gives $v_1 = v$, $v_2 = 0$. The set of the obtained Lagrangians forms *a Higgs basis Lagrangian family*, it is pictured as the grey vertical strip in fig. 1 (see [12, 15, 16]).

A. Neutral Higgs sector. General introduction

By definition η_i are standard $C-$ and $P-$ even (scalar) fields. The field

$$A = -\sin\beta\,\chi_1 + \cos\beta\,\chi_2\,, \tag{3.4}$$

is C–odd (in the interactions with fermions it behaves as $P-$ odd particle, i.e. a pseudoscalar). In other words, η_i and A are fields with opposite CP parities (see e.g. [2] for details).

The decomposition (3.1) results in the (symmetric) mass–squared matrix $\mathcal{M}$ in the η_1, η_2, A basis

$$\mathcal{M} = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{12} & M_{22} & M_{23} \\ M_{13} & M_{23} & M_{33} \end{pmatrix}, \tag{3.5a}$$

with

$$\begin{gathered}
M_{11} = \left[c_\beta^2\,\lambda_1 + s_\beta^2\,\nu + s_\beta^2 \operatorname{Re}(\lambda_{67} + 2\tilde\lambda_{67})\right]v^2, \\
M_{22} = \left[s_\beta^2\,\lambda_2 + c_\beta^2\,\nu + c_\beta^2 \operatorname{Re}(\lambda_{67} - 2\tilde\lambda_{67})\right]v^2, \\
M_{33} = \left[\nu - \operatorname{Re}(\lambda_5 - \lambda_{67})\right]v^2, \\
M_{12} = -\left[\nu - \lambda_{345} - 3\operatorname{Re}\lambda_{67}\right]c_\beta s_\beta v^2, \\
M_{13} = -\left[\delta + \operatorname{Im}\tilde\lambda_{67}\right]s_\beta v^2, \\
M_{23} = -\left[\delta - \operatorname{Im}\tilde\lambda_{67}\right]c_\beta v^2,
\end{gathered} \tag{3.5b}$$

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

$$M_A^2 = M_{33} = \left[\nu - \operatorname{Re}(\lambda_5 - \lambda_{67})\right]v^2. \tag{3.5c}$$

The masses squared M_i^2 of the physical neutral states h_i 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 $\mathcal{M}$:

$$\begin{gathered}\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R \begin{pmatrix} \eta_1 \\ \eta_2 \\ A \end{pmatrix}, \\ \text{with} \quad R\mathcal{M}R^T = diag(M_1^2,\, M_2^2,\, M_3^2)\,. \end{gathered} \tag{3.6}$$

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 $c_i = \cos\alpha_i$, $s_i = \sin\alpha_i$):

$$\begin{gathered}
R = R_3 R_2 R_1, \quad R_1 = \begin{pmatrix} c_1 & s_1 & 0 \\ -s_1 & c_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\
R_2 = \begin{pmatrix} c_2 & 0 & s_2 \\ 0 & 1 & 0 \\ -s_2 & 0 & c_2 \end{pmatrix}, \quad R_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_3 & s_3 \\ 0 & -s_3 & c_3 \end{pmatrix},
\end{gathered} \tag{3.7a}$$

$$\begin{gathered}
R = \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \equiv \\
\begin{pmatrix} c_1\,c_2 & c_2\,s_1 & s_2 \\ -c_1\,s_2\,s_3 - c_3\,s_1 & c_1\,c_3 - s_1\,s_2\,s_3 & c_2\,s_3 \\ -c_1\,c_3\,s_2 + s_1\,s_3 & -c_1\,s_3 - c_3\,s_1\,s_2 & c_2\,c_3 \end{pmatrix}.
\end{gathered} \tag{3.7b}$$

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

In general, the obtained Higgs eigenstates h_i (3.6) have no definite CP parity since they are mixtures of fields η_i and A having opposite CP parities. This provides a CP nonconservation within the Higgs sector. The interaction of these bosons with matter explicitly violates the CP–symmetry. Such mixing (and violation of CP) is absent if $M_{13} = M_{23} = 0$.

B. 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 rotation matrix R_1. It results in the neutral, CP-even Higgs fields which we denote as h and[1] $(-H)$, while the CP–odd field A remains unmixed, so that

$$\begin{pmatrix} h \\ -H \\ A \end{pmatrix} = R_1 \begin{pmatrix} \eta_1 \\ \eta_2 \\ A \end{pmatrix} \quad \text{with}$$
$$R_1 \mathcal{M} R_1^T = \mathcal{M}_1 \equiv \begin{pmatrix} M_h^2 & 0 & M'_{13} \\ 0 & M_H^2 & M'_{23} \\ M'_{13} & M'_{23} & M_A^2 \end{pmatrix}. \tag{3.8}$$

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 calculations and discussion. In the case of CP conservation (which is 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 $\alpha \in (-\pi/2, \pi/2)$,

$$\alpha = \alpha_1 - \pi/2\,, \tag{3.9}$$

which is customary for the CP–conserving case. With this notation we have

$$\begin{aligned} H &= \cos\alpha\,\eta_1 + \sin\alpha\,\eta_2, \\ h &= -\sin\alpha\,\eta_1 + \cos\alpha\,\eta_2. \end{aligned} \tag{3.10a}$$

The diagonalization of the respective $\langle 12 \rangle$ corner of mass-squared matrix $\mathcal{M}$ (3.5) results in

$$\begin{aligned} M_{h,H}^2 &= \frac{1}{2}\left(M_{11} + M_{22} \mp \mathcal{N}\right), \\ \mathcal{N} &= \sqrt{(M_{11} - M_{22})^2 + 4M_{12}^2}. \end{aligned} \tag{3.10b}$$

C. Complete diagonalization

The above diagonalization keeps in general two off-diagonal elements in matrix $\mathcal{M}_1$ (3.8):

$$\begin{gathered} M'_{13} = c_1 M_{13} + s_1 M_{23} = \\ -[\delta\cos(\beta+\alpha) - Im\tilde{\lambda}_{67}\cos(\beta-\alpha)]v^2, \\ M'_{23} = -s_1 M_{13} + c_1 M_{23} = \\ [\delta\sin(\beta+\alpha) - Im\tilde{\lambda}_{67}\sin(\beta-\alpha)]v^2. \end{gathered} \tag{3.11}$$

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 CP symmetry. Therefore the complexity of some parameters of potential in its *real vacuum form* is necessary and sufficient condition for CP violation in the Higgs sector. For the other form of Lagrangian (i.e. not for the real vacuum form) this necessary and sufficient condition for CP violation in the Higgs sector can be expressed as a requirement of complexity of combinations (which are invariant under rephasing transformation, see (2.6))

$$\lambda_5^*(m_{12}^2)^2\,, \quad \lambda_6^* m_{12}^2\,, \lambda_7^* m_{12}^2\,. \tag{3.12}$$

Now we express physical Higgs boson states h_i via h, H, A:

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R_3 R_2 \begin{pmatrix} h \\ -H \\ A \end{pmatrix} \quad \text{with} \tag{3.13}$$

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

This relation allows to discuss a general CP violating case in terms customary for the CP conserving case, i.e. with *parameters* M_H, M_h, M_A and α. The angles α_2 and α_3 describe mixing between the CP–even states h, H and the CP–odd state A.

The squared masses M_i^2 in Eq.(3.13) are the eigenvalues of the matrix $\mathcal{M}$ (3.5). Note, that the trace of mass-squared matrix does not changed under the unitary transformations. Therefore, we have *mass sum rule*

$$\begin{aligned} M_1^2 + M_2^2 + M_3^2 &= M_h^2 + M_H^2 + M_A^2 \\ &= M_{11} + M_{22} + M_{33}\,. \end{aligned} \tag{3.14}$$

D. Some cases of CP violation

Here we present some important cases.

- If $\boldsymbol{\delta = 0}$ **and** $\mathbf{Im}\,\boldsymbol{\tilde{\lambda}_{67} = 0}$, CP symmetry is not violated: h, H and A are physical Higgs bosons, with masses given by eqs. (3.10b) and (3.5c), and $\alpha_2 = \alpha_3 = 0$.
- If $\boldsymbol{\varepsilon_{13} = |M'_{13}/(M_A^2 - M_h^2)| \ll 1}$ 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 residual $\langle 23 \rangle$ corner of mass matrix (3.8) with the aid of rotation matrix R_3 (3.7a) gives states h_2 and h_3 — superpositions of H and A states with mixing angle α_3, given by

$$\tan 2\alpha_3 \approx \frac{-2M'_{23}}{M_A^2 - M_H^2}\,, \quad \alpha_2 \approx 0 \tag{3.15a}$$

.

If $M_A \approx M_H$, the CP violating mixing can be strong even at small M'_{23}/v^2, the states h_2 and h_3 may have no definite CP parity and the mass difference $M_2^2 - M_3^2$ larger than $|M_H^2 - M_A^2|$. For example, at

[1] Sign minus is needed in order to match a standard convention used for CP-conserving case, see e.g. [2].

$M_H \approx 300$ 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, $\sin 2\alpha_3 \approx 0.8$.

• If $\boldsymbol{\varepsilon_{23} = |M'_{23}/(M_A^2 - M_H^2)| \ll 1}$, 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 $\langle 13 \rangle$ minor of mass matrix (3.8) with the aid of rotation matrix R_2 (3.7a) gives states h_1 and h_3 — superpositions of h and A states with mixing angle α_2, given by

$$\tan 2\alpha_2 \approx \frac{-2M'_{13}}{M_A^2 - M_h^2}\,, \quad \alpha_3 \approx 0. \tag{3.15b}$$

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

• **Case of weak CP violation** combines both cases (3.15). If both $|M'_{13}| \ll |M_A^2 - M_h^2|$ and $|M'_{23}| \ll |M_A^2 - M_H^2|$, CP–even states h, H are weakly mixed with the CP–odd state A and parameters α_2 and α_3 are simultaneously small:

$$\begin{aligned}\tan\alpha_2 \approx s_2 \approx \frac{-M'_{13}}{M_A^2 - M_h^2} \approx \alpha_2\,,\\ \tan\alpha_3 \approx s_3 \approx \frac{-M'_{23}}{M_A^2 - M_H^2} \approx \alpha_3.\end{aligned} \tag{3.16a}$$

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

$$\begin{aligned}M_1^2 = M_h^2 - s_2^2(M_A^2 - M_h^2),\\ M_2^2 = M_H^2 - s_3^2(M_A^2 - M_H^2),\end{aligned} \tag{3.16b}$$

with M_3 given by the sum rule (3.14).

• The case of **intense coupling regime** with $M_A \approx M_h \approx M_H$ [19] may also give strong CP violating mixing even with small δ and $\mathrm{Im}\,\tilde\lambda_{67}$.

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 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. [28] and references therein).

E. Couplings to gauge bosons

The gauge bosons W and Z couple only to the CP–even fields η_1, η_2. For the physical Higgs bosons h_i (3.6) one obtains simple expressions for their couplings, which in terms of relative couplings (1.3) read

$$\begin{aligned}\chi_V^{(i)} = \cos\beta\, R_{i1} + \sin\beta\, R_{i2},\\ i = 1,2,3, \quad \text{and } V = W \text{ or } Z.\end{aligned} \tag{3.17a}$$

Note that due to the unitarity of transformation matrix R, the following sum rule takes place [20]

$$\sum_{i=1}^{3} (\chi_V^{(i)})^2 = 1\,. \tag{3.17b}$$

IV. YUKAWA INTERACTIONS

A. General discussion

In the general case the Yukawa Lagrangian reads

$$\begin{aligned}-\mathcal{L}_{\mathrm{Y}} = \bar Q_L[(\Gamma_1\phi_1 + \Gamma_2\phi_2)d_R\\ +(\Delta_1\tilde\phi_1 + \Delta_2\tilde\phi_2)u_R] + \text{h.c.},\end{aligned} \tag{4.1}$$

plus 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 the right-handed field singlets (with $q_{\mathrm{L}} = (1-\gamma_5)q/2$), $\tilde\phi_a = i\tau_2\phi_a^{\dagger\mathrm{T}}$. The matrices Γ and Δ are 3–dimensional matrices in the family space with generally complex coefficients.

Obviously the reparametrization transformation (2.2) induces changes in 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 ϕ_i by the following transformations of fermion fields

$$\begin{aligned}Q_{Lk} \to Q_{Lk}e^{i\tau_{qk}}, \;\; d_{Rk} \to d_{Rk}e^{i(\tau_{qk}+\tau_{dk})},\\ u_{Rk} \to u_{Rk}e^{i(\tau_{qk}+\tau_{uk})}.\end{aligned} \tag{4.2a}$$

The corresponding transformation of the parameters of Yukawa Lagrangian supplemented transformation (2.6) have form

$$\Gamma_i \;\to\; \Gamma_i \begin{pmatrix} e^{i\tau_{d1}} \\ e^{i\tau_{d2}} \\ e^{i\tau_{d3}} \end{pmatrix} e^{\mp i\rho_i} \;\; \text{with} \begin{array}{c} -\;\; for \;\; i=1,\\ +\;\; for \;\; i=2 \end{array} \tag{4.2b}$$

and similar for Δ_i.

An existence in the Yukawa couplings of the off-diagonal (in family index) terms results in the flavor-changing neutral-currents (FCNC). The rephasing invariance (2.6), (4.2) 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 m_{12}^2 and λ's).

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 counter terms 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 [8], [21]. Therefore ([4, 22]), to have only the soft violation of Z_2 symmetry (to prevent $\phi_1 \leftrightarrow \phi_2$ transitions at small distances), we demand that

$$\begin{array}{c}\textit{each right-handed fermion couple}\\ \textit{to only one scalar field, either } \phi_1 \text{ or } \phi_2.\end{array} \tag{4.3}$$

For example, the case $\Gamma_2 = \Delta_1 = 0$ with diagonal Γ_1, Δ_2 corresponds to Model II, while $\Gamma_2 = \Delta_1 = 0$ – to Model I (see e.g. [2]). The rephasing transformations (2.6), (4.2) with different phases generate from one Lagrangian of Model II (or I) *the Model II (or I) Lagrangians family* in which the property (4.3) is explicitly seen (general reparametrization transformation (2.2) makes this property latent). If the Model II (or I) family coincides with the soft Z_2 violated Lagrangian family (crossed vertical strip in Fig. 1), these properties (soft Z_2 violation and (4.3)) are stable under radiative corrections.

If mentioned families of Lagrangians exist but don't coincide, the loop corrections transform our Lagrangian to that of true hard violated Z_2 symmetry. The appearance of counter–terms, leading to hard violating Z_2 symmetry, requires adding of the corresponding terms in the initial Lagrangian, similar to that it was discussed in sec. II B in context of the mixed kinetic term.

B. Model II

We limit ourselves to the discussion of Model II, 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 rephasing transformation (2.5) induces only changes of phases of Yukawa couplings, keeping mentioned basic property of Model II immutable. The reparameterization transformation (2.2) generally makes above property hidden just as in the case of soft Z_2 violation. We use below also *real vacuum form of Lagrangian*, This form corresponds to the intersection of crossed and black strips in fig. 1.

Using matrices $\Gamma_1 = diag(g_{d1}, g_{d2}, g_{d3})$ and $\Delta_2 = diag(g_{u1}, g_{u2}, g_{u3})$ (like in MSSM) with real g_i, as mentioned above, we get

$$\begin{aligned}-\mathcal{L}_Y^{II} = &\sum_{k=1,2,3} \bar{Q}_{Lk}\left[g_{dk}\phi_1 d_{Rk} + g_{uk}\tilde{\phi}_2 u_{Rk}\right]\\ &+ \sum_{k=1,2,3} g_{\ell k}\bar{\ell}_{Lk}\phi_1\ell_{Rk} + \text{h.c.}\end{aligned} \tag{4.4}$$

For the interaction of the charged Higgs bosons e.g. with t-quark, the Lagrangian (4.4) gives

$$\begin{aligned}\mathcal{L}_{H^-tb} = &\frac{M_t}{v\sqrt{2}}\cot\beta\,\bar{b}(1+\gamma^5)H^- t\\ &+\frac{M_b}{v\sqrt{2}}\tan\beta\,\bar{b}(1-\gamma^5)H^- t + h.c.\end{aligned} \tag{4.5}$$

Since v.e.v.'s of scalar fields are responsible for the fermion mass similarly as in the SM, the relative Yukawa couplings of 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 (3.6):

$$\begin{aligned}\chi_u^{(i)} &= \frac{1}{\sin\beta}[R_{i2} - i\cos\beta\, R_{i3}],\\ \chi_d^{(i)} &= \frac{1}{\cos\beta}[R_{i1} - i\sin\beta\, R_{i3}].\end{aligned} \tag{4.6}$$

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

In the particular case of weak CP violation (with small s_2, s_3 (3.16)) these relative couplings together with the corresponding ones to gauge bosons are presented in Table I.

TABLE I: *Basic relative couplings in the weak CP-conserving case. The upper lines correspond the case with no CP violation and second lines (in parenthesis) contain the correction terms $\propto s_2$, s_3.*

	χ_V	χ_u	χ_d
h_1	$\sin(\beta-\alpha)$ $(+0)$	$\dfrac{\cos\alpha}{\sin\beta}$ $(-is_2\cot\beta)$	$-\dfrac{\sin\alpha}{\cos\beta}$ $(-is_2\tan\beta)$
h_2	$-\cos(\beta-\alpha)$ $(+0)$	$-\dfrac{\sin\alpha}{\sin\beta}$ $(-is_3\cot\beta)$	$-\dfrac{\cos\alpha}{\cos\beta}$ $(+is_3\tan\beta)$
h_3	0 $(-s_2\sin(\beta-\alpha) + s_3\cos(\beta-\alpha))$	$-i\cot\beta$ $(+s_3\dfrac{\cos\alpha}{\sin\beta} - s_2\dfrac{\sin\alpha}{\sin\beta})$	$-i\tan\beta$ $(+s_2\dfrac{\sin\alpha}{\cos\beta} + s_3\dfrac{\cos\alpha}{\cos\beta})$

- In the case of no CP violation one can express the triple Higgs couplings via relative couplings of

Higgs bosons to gauge bosons and fermions. Denoting by ϕ either h or H, we find

$$g_{\phi\phi\phi}=\frac{3}{2v}\left[\left(\chi_u^\phi+\chi_d^\phi-\chi_V^\phi\chi_u^\phi\chi_d^\phi\right)(M_\phi^2-\nu v^2)+\chi_V^\phi\nu v^2\right],$$

$$\forall\phi_1\neq\phi_2\;\Rightarrow\; g_{\phi_1\phi_2\phi_2}=-\frac{1}{2v}\chi_V^{\phi_1}\left[\chi_u^{\phi_2}\chi_d^{\phi_2}(2M_{\phi_2}^2+M_{\phi_1}^2-3\nu v^2)-\nu v^2\right],$$

$$g_{\phi AA}=\frac{1}{v}\left[(2M_A^2-M_\phi^2)\chi_V^\phi+(M_\phi^2-\nu v^2)(\chi_u^\phi+\chi_d^\phi)\right],\tag{4.7}$$

$$g_{A\phi_1\phi_2}=g_{AAA}=g_{AH^+H^-}=0\,,$$

$$g_{\phi H^+H^-}=\frac{1}{v}\left[\left(2M_{H^\pm}^2-M_\phi^2\right)\chi_V^\phi+(M_\phi^2-\nu v^2)(\chi_u^\phi+\chi_d^\phi)\right].$$

(These results are valid also in the case of weak CP violation).

C. Useful relations in Model II

The unitarity of the mixing matrix R allows to obtain a number of useful relations [20, 23, 24] between the relative couplings of neutral Higgs particles to gauge bosons (3.17a) and fermions (4.6) (*basic relative couplings*), which can be treated as measurable quantities.

1. *The pattern relation* among basic relative couplings holds of *each neutral Higgs particle* h_i [23, 24]:

$$(\chi_u^{(i)}+\chi_d^{(i)})\chi_V^{(i)}=1+\chi_u^{(i)}\chi_d^{(i)}\,.\tag{4.8}$$

2. The relations (4.6) allow also to write for each neutral Higgs boson h_i *a horizontal sum rule* [25]:

$$|\chi_u^{(i)}|^2\sin^2\beta+|\chi_d^{(i)}|^2\cos^2\beta=1\,.\tag{4.9}$$

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 [25].

3. *A vertical sum rule* for each relative coupling χ_j for *all three neutral Higgs bosons h_i is given by*:

$$\sum_{i=1}^{3}(\chi_j^{(i)})^2=1\qquad (j=V,d,u)\,.\tag{4.10}$$

4. Besides, the useful *linear relation* follows directly from Eqs. (3.17a), (4.6):

$$\begin{gathered}\chi_V^{(i)}=\cos^2\beta\,\chi_d^{(i)*}+\sin^2\beta\,\chi_u^{(i)}=\\=\cos^2\beta\,\chi_d^{(i)}+\sin^2\beta\,\chi_u^{(i)*}\Rightarrow\\ \begin{cases}\chi_V^{(i)}=\mathrm{Re}\left(\cos^2\beta\chi_d^{(i)}+\sin^2\beta\chi_u^{(i)}\right),\\ \mathrm{Im}\left(\cos^2\beta\chi_d^{(i)}-\sin^2\beta\chi_u^{(i)}\right)=0.\end{cases}\end{gathered}\tag{4.11}$$

By excluding from (4.11) the parameter β (with the aid of the (4.9)), one obtains a new relation:

$$(1-|\chi_d^{(i)}|^2)\,\mathrm{Im}\,\chi_u^{(i)}+(1-|\chi_u^{(i)}|^2)\,\mathrm{Im}\,\chi_d^{(i)}=0\,.\tag{4.12}$$

The relations (4.8), (4.10), (4.12) *are reparametrization independent* while (4.9) and (4.11) take place only for the Model II form of Lagrangian.

5. One can also express $\tan\beta$, which is a basic parameter of the 2HDM defined for the Model II Lagrangian family, via the basic relative couplings:

$$\tan^2\beta=\frac{(\chi_V^{(i)}-\chi_d^{(i)})^*}{\chi_u^{(i)}-\chi_V^{(i)}}=\frac{\mathrm{Im}\,\chi_d^{(i)}}{\mathrm{Im}\,\chi_u^{(i)}}=\frac{1-|\chi_d^{(i)}|^2}{|\chi_u^{(i)}|^2-1}.\tag{4.13}$$

d. Some applications. Let us remind that the relative couplings to quarks are generally complex while coupling to gauge bosons are real.

- From (4.9) we get that,

$$\begin{array}{ll}\textit{if} & |\chi_u^{(i)}|\gg 1\;\Rightarrow\;\tan\beta\ll 1\,;\\ \textit{if} & |\chi_d^{(i)}|\gg 1\;\Rightarrow\;\tan\beta\gg 1\,.\end{array}\tag{4.14}$$

It is instructive to consider now consequences of the relations (4.8)–(4.10) for the case when some basic relative couplings of a Higgs boson are close to ±1.

- In virtue of (4.9) for moderate $\tan\beta$ we have

$$\textit{if}\ |\chi_u^{(i)}|\approx 1\;\Rightarrow\;|\chi_d^{(i)}|\approx 1.\tag{4.15}$$

Note, that if $\tan\beta$ is extremely large or extremely small, *horizontal sum rule* allows $|\chi_d^{(i)}|$ to differ strong from 1 or $|\chi_u^{(i)}|$ to differ strong from 1, respectively (in agreement with (4.14)).

- From (4.10),

$$\begin{array}{ll}\textit{if} & \chi_u^{(2)}\approx\pm1\;\Rightarrow\;\chi_u^{(1)}\approx\pm i\chi_u^{(3)}\,,\\ \textit{if} & \chi_d^{(2)}\approx\pm1\;\Rightarrow\;\chi_d^{(1)}\approx\pm i\chi_d^{(3)}\,.\end{array}\tag{4.16}$$

- For $\chi_V^{(2)}\sim\pm1$ (analogously for h_1 and h_3)

$$\begin{gathered}\textit{if}\quad \chi_V^{(2)}\approx\pm1\\ \Rightarrow\begin{cases}(a)\;\; \chi_u^{(2)}\approx\chi_V^{(2)}\;\;\textit{or}\;\;\chi_d^{(2)}\approx\chi_V^{(2)}\,,\\ (b)\;\; \chi_u^{(2)}\approx\chi_d^{(2)}\approx\chi_V^{(2)}\,,\\ (c)\;\; \chi_V^{(1)}\approx\chi_V^{(3)}\approx 0\,,\\ (d)\;\; \chi_u^{(1)}\chi_d^{(1)}\approx\chi_u^{(3)}\chi_d^{(3)}\approx -1\,.\end{cases}\end{gathered}\tag{4.17}$$

The property (a) obtained from (4.8b), means that the coupling of h_2 to at least one fermion type is close to the $\chi_V^{(2)}$. The property (b) follows from property (a) and (4.11), at moderate $\tan\beta$. The fact that the couplings of Higgs bosons to gauge bosons are real leads, with the aid of (4.10), in the property (c). Taking into account property (c) and the pattern relation (4.8a) 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, properties similar to (4.16), (4.17) take place as well in the cases when $\chi_i^{(1)} \approx \pm 1$ or $\chi_i^{(3)} \approx \pm 1$.)

V. CONSTRAINTS FOR HIGGS LAGRANGIAN

A. Positivity (vacuum stability) and minimum constraints

• To have a *stable vacuum*, the potential must be positive at large quasi–classical values of fields $|\phi_i|$ (*positivity constraints*) for an arbitrary direction in the (ϕ_1, ϕ_2) plane. Let $(\phi_1^\dagger \phi_1) = x_1 \geq 0$, $(\phi_2^\dagger \phi_2) = x_2 \geq 0$. Than $(\phi_1^\dagger \phi_2) = \sqrt{x_1 x_2}\, c e^{i\phi}$ with $|c| \leq 1$ (due to Schwartz theorem). In the case of soft Z_2 violation the potential is the quadratic form in x_1, x_2. It should be positive at large x_i at different c and ϕ. This condition gives (see e.g. [26, 27, 29, 30])

$$\begin{gathered}\lambda_1 > 0\,, \quad \lambda_2 > 0, \;\; \lambda_3 + \sqrt{\lambda_1 \lambda_2} > 0, \\ \lambda_3 + \lambda_4 - |\lambda_5| + \sqrt{\lambda_1 \lambda_2} > 0.\end{gathered} \tag{5.1}$$

(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 ϕ in respect to the phase of λ_5 we obtain the latter constraint.)

• The condition for vacuum (2.10) describes the *extremum* of potential but not obligatory the minimum. The *minimum constraints* are the conditions ensuring that above extremum is a local minimum for all directions in (ϕ_1, ϕ_2) space, except 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 mean that its eigenvalues, the physical mass squared, are positive: $M_{h_i}^2$, $M_{H^\pm}^2 > 0$.

B. Unitarity constraints

The quartic terms of Higgs potential are transformed to the quartic self–couplings of the physical Higgs bosons. They lead, in the tree approximation, to s–wave Higgs-Higgs and $W_L W_L$ and $W_L H$, 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 in the minimal SM, with one Higgs doublet and Higgs potential $V = (\lambda/2)(\phi^\dagger\phi - v^2/2)^2$ [4]. In this model Higgs-boson mass $M_H = v\sqrt{\lambda}$; its width Γ_H grow with M_H as M_H^3. Unitarity limit corresponds simultaneously the case when $\Gamma_H \approx M_H$, so that the physical Higgs boson disappears, besides the strong interaction in the Higgs sector is realized for $\sqrt{s} > v\sqrt{\lambda} \gtrsim v\sqrt{8\pi} \approx 1.2$ TeV, as a strong interaction of W_L and Z_L. Therefore, the unitarity limit is a boundary (in the λ space) between two physical regimes. Below the unitarity limit we have more or less narrow Higgs boson with well known properties. Above the unitarity limit the Higgs boson disappears as a particle and strong interaction in the Higgs sector becomes essential.

Akeroyd *et al.* [31] 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 the parameter λ_5 is complex. The application of rephasing transformation (2.5) allows to eliminate 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 one of this Lagrangian allows to extend the above results to the CP nonconserving case [27]. It is useful to present unitarity constraints as the bounds for the eigenvalues $\Lambda_{Y\sigma}^{Z_2 parity}$ 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 [27]:

$$\begin{gathered}|\Lambda_{Y\sigma\pm}^{Z_2}| < 8\pi \qquad \textit{with} \\ \Lambda_{21\pm}^{even} = \frac{1}{2}\left(\lambda_1 + \lambda_2 \pm \sqrt{(\lambda_1 - \lambda_2)^2 + 4|\lambda_5|^2}\,\right), \\ \Lambda_{21}^{odd} = \lambda_3 + \lambda_4\,, \quad \Lambda_{20}^{odd} = \lambda_3 - \lambda_4\,, \\ \Lambda_{01\pm}^{even} = \frac{1}{2}\left(\lambda_1 + \lambda_2 \pm \sqrt{(\lambda_1 - \lambda_2)^2 + 4\lambda_4^2}\right), \\ \Lambda_{01\pm}^{odd} = \lambda_3 \pm |\lambda_5|\,, \\ \Lambda_{00\pm}^{even} = \frac{3(\lambda_1 + \lambda_2) \pm \sqrt{9(\lambda_1 - \lambda_2)^2 + 4(2\lambda_3 + \lambda_4)^2}}{2}, \\ \Lambda_{00\pm}^{odd} = \lambda_3 + 2\lambda_4 \pm 3|\lambda_5|\,.\end{gathered} \tag{5.2}$$

At small ν these constraints result in moderately large upper bound of $600 \div 700$ GeV for M_H, M_A, $M_{H^\pm}$ (see examples in Table II of sec. VI B), see also e.g. [31] for CP conserving case. At large ν, all M_H, M_A, $M_{H^\pm}$ can be large without violation of unitary constraints (5.2).

The correspondence between a violation of the tree-level unitarity limit and a lack of realization of the Higgs field as a particle, like in the minimal SM, takes place in the 2HDM only in the case when *all* constraints (5.2) are violated simultaneously. If only some of these constraints are violated the physical picture become more complex.

C. 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 (5.1) are valid for some particular directions of growth of quasi-classic fields ϕ. Similarly, unitarity constraints (5.2) hold for such transition amplitudes which don't violate Z_2 symmetry.

With hard violation of Z_2 symmetry one should consider new directions in the ϕ_i phase space, which violate the Z_2 symmetry. Moreover, an existence of the $\varkappa$ term makes some directions in the λ's parameter space equivalent, because different sets of these parameters can be obtained from each other by transformations like (2.9). This subject is beyond a scope of this paper.

VI. 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 and other Higgs bosons escape observation since they are too heavy. Besides, many authors assume **in addition** that masses of other Higgs bosons M are close to the scale of new physics, and the theory should possess an explicit decoupling property [32], *i.e. the correct description of the observable phenomena must be valid for the unphysical limit* $M \to \infty$ [30, 33–36]. However, the 2HDM allows also for another realization of the mentioned SM–like physical picture.

A. Decoupling of heavy Higgs bosons

In 2HDM the decoupling case corresponds to

$$\nu \gg |\lambda_i|\,. \tag{6.1}$$

In this case equations for masses and mixing angles α_i simplify. With accuracy up to λ/ν terms we obtain first the masses of the subsidiary Higgs states obtained at the first stage of diagonalization (3.8-3.11). From eqs. (3.10b) we derive

$$\begin{aligned}
\frac{M_h^2}{v^2} &= \underbrace{c_\beta^4\lambda_1 + s_\beta^4\lambda_2 + 2s_\beta^2c_\beta^2\lambda_{345}}_{soft} + \underbrace{8s_\beta^2c_\beta^2\,\mathrm{Re}\,\lambda_{67}}_{hard},\\
\frac{M_H^2}{v^2} &= \underbrace{\nu + s_\beta^2c_\beta^2(\lambda_1+\lambda_2-2\lambda_{345})}_{soft}\\
&-\underbrace{[2(c_\beta^2-s_\beta^2)\,\mathrm{Re}\,\tilde\lambda_{67} + (8s_\beta^2c_\beta^2-1)\,\mathrm{Re}\,\lambda_{67}]}_{hard}.
\end{aligned} \tag{6.2}$$

In the proper decoupling limit $\nu \to \infty$ we have $\beta-\alpha \to \pi/2$. It is useful to characterize a deviation from this limiting value by introducing 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. (3.10):

$$\Delta_{\beta\alpha} = -\frac{L_a s_{2\beta}}{2\nu}\,, \tag{6.3}$$

$$L_a = \underbrace{s_\beta^2\lambda_2 - c_\beta^2\lambda_1 + c_{2\beta}\lambda_{345}}_{soft} + \underbrace{2\,\mathrm{Re}\,(2c_{2\beta}\lambda_{67} - \tilde\lambda_{67})}_{hard}.$$

The lightest Higgs boson h_1. The condition (6.1) together with constraint (2.15) shows that the element M'_{13} of the matrix (3.8), 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 $s_2 \sim |\lambda|/\nu$ (3.16a).

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 Model II as in the SM (with accuracy $|\lambda|/\nu$). Besides, h_1 practically decouples from $H^\pm$, since the quantity $\chi_{H^\pm}^{(1)} = g_{H^\pm}^h v/M_{H^\pm}^2 \sim \mathcal{O}(|\lambda|/\nu)$ (4.7).

Higgs bosons h_2, h_3 and $H^\pm$. The Eqs. (3.2), (3.5c), (6.2) show that $M_{H^\pm}^2 \approx M_A^2 \approx M_H^2 = v^2\nu\left[1+\mathcal{O}\left(\frac{|\lambda|}{\nu}\right)\right]$, i.e. $H^\pm$, H and A (and therefore h_2 and h_3) are very heavy and almost degenerate in masses,

$$M_{H^\pm}^2 \approx M_2^2 \approx M_3^2 \approx v^2\nu\left[1+\mathcal{O}\left(\frac{|\lambda|}{\nu}\right)\right]. \tag{6.4}$$

That is one of the reasons to consider the condition of the decoupling regime (6.1)) in the form, used e.g. in ref. [30], $M_A^2 \gg |\lambda|v^2$.

In the considered case the CP violating mixing between H and A can be strong, i.e. mixing angle α_3 given by Eq. (3.15a) can be large as it was discussed in sec. III D.

Since $\chi_V^{(h)} \approx 1$, coupling of H to gauge bosons is very small, while A does not couple to gauge bosons (Table I). With mixing between H, A states given by angle α_3, we have from (6.2)

$$\begin{array}{l}
\chi_V^{(H)} = \cos(\beta-\alpha) \approx \Delta_{\beta\alpha}\,,\ \ \chi_V^{(A)} = 0\ \Rightarrow\\
\chi_V^{(2)} \approx -\cos\alpha_3\,\Delta_{\beta\alpha},\ \ \chi_V^{(3)} \approx \sin\alpha_3\,\Delta_{\beta\alpha}.
\end{array} \tag{6.5a}$$

Besides, couplings of H and A to u- and d-type quarks coincide in their modules (see Table I), so that also the corresponding couplings for $h_{2,3}$ 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. (4.6) and (3.7) we obtain

$$\begin{array}{l}
\chi_u^{(2)} = i\chi_u^{(3)} = \cot\beta\, e^{-i\alpha_3},\\
\chi_d^{(2)} = -i\chi_d^{(3)} = -\tan\beta\, e^{i\alpha_3}.
\end{array} \tag{6.5b}$$

The corresponding Higgs decay widths are given mainly by fermions,

$$\begin{array}{c}
\Gamma_A \approx \Gamma_H \approx \Gamma_2 \approx \Gamma_3\\
= \dfrac{3}{16\pi}\cot^2\beta\left[1+\dfrac{m_b^2}{m_t^2}\tan^4\beta\right]M_H\\
\textit{with}\ \ \dfrac{\Gamma_A-\Gamma_H}{\Gamma_H} \sim \dfrac{m_t}{M_H}.
\end{array} \tag{6.5c}$$

Here we take into account that $v^2/m_t^2 \approx 2$. The gauge boson contributions to these widths are negligibly small ($\sim L_a^2/\nu$). In this case the equations for α_3, $M_{2,3}$ and $\Gamma_{2,3}$ include shift of A, H poles due to their proper widths (6.5c). The obtained mass squared matrix is non-hermitian, therefore, the mixing angle α_3 become complex, and the states h_2, h_3 non-orthogonal (see [11, 39] for more details). It is seen from the corrected eq. (3.15):

$$\tan 2\alpha_3 \approx \frac{2M'_{23}}{M_A^2 - M_H^2 - i\Delta}\,, \quad \Delta = M_A\Gamma_A - M_H\Gamma_H\,. \tag{6.6}$$

Note that with this strong overlapping of states the experimental distinguishing of states h_2, h_3 seems to be difficult. The visible effects of CP violation in the fermion interaction will be very similar in both quite different cases: of a true CP violation and of a strong overlapping of H and A states without 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 reasonable heavy, can also be realized in 2HDM for relatively small ν, i.e. beyond decoupling limit. In this case possible masses of heavy Higgses are bounded from above by unitarity constraints for λ's. In the case of CP violation the corresponding bounds can be generally enhanced since the constraints (5.2) put limit on parameter $|\lambda_5|$ while equations for masses contain $\mathrm{Re}\,\lambda_5$. For a non-decoupling case we present in Table II some particular examples of sets of parameters of potential, satisfying constraints (5.2), for light h (mass 120 GeV) and heavy H, $H^\pm$.

The first three lines presents set of λ, ν values 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 small $\tan\beta$ and reasonably small $\nu \approx (M_h/v)^2$, as well as for $\tan\beta \approx 1$, $\nu \approx 0$.

TABLE II: *Sets of parameters of potential for light h (mass 120 GeV) and heavy H, $H^\pm$ satisfying constraints (5.2) 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	-	-
0.02	6	1	5.5	-6	-6	0.24	120	600	600	600	-	-
1	6.25	6.25	6.25	-6	-6	0	120	600	600	600	-	-
10	4	8	4.4	-9	$-0.5+0.3i$	0.24	120	700	206	556	0.09	0.02

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

In the considered non-decoupling case couplings of the lightest Higgs boson to gauge bosons, quarks and leptons can be either close to their SM values or differ 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 [41], see also [23, 24]. Note that also in such case some non-decoupling effects due to heavy Higgs bosons may appear.

C. Natural set of parameters of 2HDM

First of all, we remind of our discussion of the hard violation of Z_2 symmetry. In addition to difficulties with the mixed kinetic term, in this case Yukawa sector cannot be described by simple models 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 is considered as such which corresponds to the case of softly broken Z_2 symmetry.

The eqs. (3.5), (3.8), (3.11) show explicitly that the CP violation in the Higgs sector can be weak for the arbitrary mixing angles α and β only if $\mathrm{Im}\,(m_{12}^2) \propto \delta v^2$ is small enough, i.e.

$$\mathrm{Im}\, m_{12}^2 \ll \begin{array}{ll} (a) & |M_A^2 - M_h^2|, \\ (b) & |M_A^2 - M_h^2|, |M_A^2 - M_H^2|. \end{array} \tag{6.7}$$

If the case (b) is realized, CP is weakly violated for all h_i, if the case (a) is realized, CP is weakly violated only for h_1.

This simple condition is valid only for the real vacuum form of potential, sec. II E. For all other rephasing equivalent Lagrangians the condition (6.7) becomes more complex including both $\mathrm{Im}\, m_{12}^2$ and

$\mathrm{Re}\, m_{12}^2$. The generalization of the condition (6.7) should be formulated independently on the rephasing parameter. Therefore, for *the natural set of parameters of 2HDM* we require that both $\mathrm{Im}\, m_{12}^2$ and $\mathrm{Re}\, m_{12}^2$ are small for all rephasing equivalent Lagrangians. In virtue of (2.14), (2.15), (3.11) in the case of soft violation of Z_2 symmetry the same requirements should be transmitted to $\mathrm{Re}\,\lambda_5$ and $\mathrm{Im}\,\lambda_5$. It means that we define a *natural set of parameters* as follows

$$|\nu|,\ |\lambda_5| \ll |\lambda_{1-4}|\,. \tag{6.8}$$

Contrary, in the decoupling case, where h_1 can differ from h by a small admixture of A (while H and A can still be mixed strong) the term m_{12}^2 has the *unnatural property*, namely $\mathrm{Re}\, m_{12}^2 \gg \mathrm{Im}\, m_{12}^2$. From this point of view *the decoupling case of 2HDM (6.1) is unnatural*.

For the natural set of parameters of 2HDM the breaking of the Z_2 symmetry is governed by a small parameter (ν). Due to 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 at the loop level. In this respect we use term *natural* in the same sense as in ref. [5].

In accordance with Eq. (3.5), for the natural set of parameters also M_A cannot be too large (see Table II). This opportunity is not ruled out by data.

VII. SUMMARY

• In our approach we introduce *the 16-dimensional space of Lagrangians with coordinates given by the Lagrangian parameters*. Within this space there is the 3-dimensional subspace – *the reparametrization equivalent space*, containing Lagrangians which can be obtained from a chosen one by the reparametrization transformations (2.3). All the Lagrangians from this subspace describe the same physical reality. Different properties of physical model can either be explicit or hidden for different families of Lagrangians in the mentioned reparametrization equivalent space. Different forms 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 reparametrization invariant while many other parameters of theory (like $\tan\beta$) are reparametrization dependent.

The reparametrization equivalent space is naturally sliced to *the rephasing equivalent subspaces*, which are described by transformations (2.2) with $\theta = 0$ (the rephasing transformations) 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 Higgs sector leads to an existence of physical neutral Higgs bosons without a definite CP parity. The necessary condition for such CP violation is that some of coefficients of the Higgs Lagrangian are complex. However, complex parameters can appear also in the CP conserving case if an unappropriate reparametrization form of Lagrangian is chosen. We found a specific, *real vacuum form of Lagrangian* in which complexity of the parameters of Higgs Lagrangian becomes a necessary condition for the CP violation in Higgs sector. This condition is also sufficient for the CP violation in Higgs sector, except for very specific relations among mentioned imaginary parts.

• The 2HDM provides 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) and various levels 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 m_{12}^2 in the Higgs potential. In this case doublets ϕ_1 and ϕ_2 mix near EWSB scale but they don't mix at smaller distances. The reparametrization transformation converts such Higgs Lagrangian $\mathcal{L}_s$, to the form which looks like a general Lagrangian with terms as for a hard violation of the Z_2 symmetry (*hidden soft Z_2 violation form of Lagrangians*). However, in this case the parameters of Higgs potential are related 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 a 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 loop corrections from hard terms of a Higgs potential. We did not find a fully consistent formulation of 2HDM in the case when 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 violation of Z_2 symmetry. Nevertheless, our discussion of a hard violation of Z_2 symmetry is incomplete just as all other analyses known to us, since effects related to the running coefficient of the mixed kinetic term should be analysed 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. 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 the real vacuum Lagrangian. We use in our analysis this very form of Lagrangian. We prefer to express the mass terms of Higgs potential via v.e.v.'s, $v_{1,2}$ and the free dimensionless parameter $\nu \propto \mathrm{Re}\, m_{12}^2$, (2.14).

The particular form of Lagrangian written for fields ϕ_i is reparametrization dependent. On the contrary the description of Lagrangian in terms of the observable Higgs states h_i is reparametrization invariant. For the neutral Higgs sector, the transition 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 our real vacuum form of Lagrangian this step is identical to the one used in the CP conserving case. It allows to describe the general CP violating case in terms of well known states h, H and A treated here 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 the real vacuum form of Lagrangian is necessary and sufficient condition for the CP violation in Higgs sector. Our procedure allows to analyze easily various important cases when one of neutral Higgs boson is almost the CP-even one, while two other neutral Higgs bosons can strongly mix, leading to a strong CP violation in the processes with exchange of these Higgs bosons.

• Considering the Yukawa interactions we note that for a case of hard violation of Z_2 symmetry the most general form of this interaction (e.g. Model III) should be implemented. We limit ourselves to models in which each fermion isosinglet couples to only one Higgs field and discuss the flavor structure of such couplings. Next we consider in detail the Model II, for which the well known form appears only in *the Model II Lagrangian family* defined in sec. IV. Here we assume that this family coincides with mentioned above family of Lagrangians with explicit softly violated Z_2 symmetry. In addition we use the real vacuum form of Lagrangian which corresponds in fig. 1 to the intersection of the crossed vertical strip and black horizontal strip.

• In this paper which is based on [1] we extend our approach introduced earlier for the CP conserving case in [23, 24] 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 (2.14) instead of variety of parameters λ's and mixing angles α_i, β. This way phenomenological analyses simplify considerably.

We present a series of relations between different relative couplings of each Higgs boson, (4.8)–(4.12), both the reparametrization invariant and reparametrization dependent ones. Among these relations there are well known sum rules, the pattern relation (obtained by us in [23] for the CP conserving case and in [24] for the CP violation), and new linear relations. Eq. (4.13) represents the formulae which allow to determine the quantity $\tan\beta$ for the Model II family of Lagrangians.

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 couplings in the SM (4.14)–(4.17).

• As the obtained relations between relative couplings are of great phenomenological importance it was crucial to check how the radiative corrections influence them; it was found 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, like the positivity condition or the vacuum stability condition at large quasiclassical values of ϕ_i, 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 till now only in the CP conserving case. All known results in this field were obtained for the case of soft violation of Z_2 symmetry only. We ascertained that these results are valid also in the case of hard violation of Z_2 symmetry, as a part of more general system of constraints.

• We perform the detailed discussion about 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 [24],[30] such situation can be realized in the different regions of ν. At $\nu \gg |\lambda_i|$ we have decoupling case in which the lightest Higgs boson 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 (6.5).

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 in context of the rephasing invariance. Here one can expect some non-decoupling effects due to the heavy Higgs bosons [23, 24, 37]. The detailed analysis of various SM-like realizations and some non-decoupling effects is presented in [41].

• Note that the CP violation can be implemented in a model in different ways. In this paper we consider mainly the CP violation given by complex values of some parameters of Higgs Lagrangian. However, there are other ways of implementation of CP violation. The first one, mentioned in sec. IV A rely on complex values of terms of Yukawa coupling matrices. The second way, used in fact in many analyses of MSSM is related to the CP nonconservation in the coupling of Higgs bosons to some other particles like superpartners. The general reasons of renormalizability demand to add in these cases the CP violated terms also in Higgs Lagrangian.

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