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# Tree-level unitarity constraints in the most general two Higgs doublet model

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We obtain tree-level unitarity constraints for the most general Two-Higgs-Doublet Model (2HDM) with explicit *CP*-violation. We briefly discuss correspondence between possible violation of tree-level unitarity limitation and physical content of the theory.

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## I. INTRODUCTION

### A. The two-Higgs-doublet model

The Electroweak Symmetry Breaking in the Standard Model (SM) is described usually with the Higgs mechanism. In its simplest variant, an initial Higgs field is an isodoublet of scalar fields with weak isospin $\vec{\sigma}$. The simplest extension of the Higgs sector known as two-Higgs-doublet model (2HDM) consists in introducing two Higgs weak isodoublets of scalar fields $\phi_1$ and $\phi_2$ with hypercharge $Y = +1$ (for a review, see [1,2]).

We consider the Higgs potential of 2HDM in the form

$$V = \frac{\lambda_1}{2}(\phi_1^\dagger\phi_1)^2 + \frac{\lambda_2}{2}(\phi_2^\dagger\phi_2)^2 + \lambda_3(\phi_1^\dagger\phi_1)(\phi_2^\dagger\phi_2) + \lambda_4(\phi_1^\dagger\phi_2)(\phi_2^\dagger\phi_1) + \left\{\frac{1}{2}\lambda_5(\phi_1^\dagger\phi_2)^2 + [\lambda_6(\phi_1^\dagger\phi_1) + \lambda_7(\phi_2^\dagger\phi_2)](\phi_1^\dagger\phi_2) + \text{h.c.}\right\} - \frac{1}{2}\{m_{11}^2(\phi_1^\dagger\phi_1) + [m_{12}^2(\phi_1^\dagger\phi_2) + (m_{12}^2)^*(\phi_2^\dagger\phi_1)] + m_{22}^2(\phi_2^\dagger\phi_2)\}. \quad (1)$$

Here, $\lambda_{1-4}$, $m_{11}^2$ and $m_{22}^2$ are real (due to hermiticity of the potential), while $\lambda_{5-7}$ and $m_{12}$ are, in general, complex.

This potential with real coefficients describes the theory without *CP* violation in the Higgs sector while complex values of some coefficients here make *CP* violation in Higgs sector possible (a more detailed discussion of many points here and references see in Ref. [2]).

(i) The crucial role in the 2HDM is played by the discrete $Z_2$-symmetry, i.e. symmetry under transformation

$$(\phi_1 \leftrightarrow \phi_1, \phi_2 \leftrightarrow -\phi_2) \quad \text{or} \quad (\phi_1 \leftrightarrow -\phi_1, \phi_2 \leftrightarrow \phi_2). \quad (2)$$

This symmetry forbids ($\phi_1$, $\phi_2$) mixing.

With this symmetry, the *CP* violation in the Higgs sector is forbidden and the Flavor Changing Neutral Currents (FCNC) are unnatural. In the "realistic" theory this $Z_2$ symmetry is violated.

Potential (1) contains the $m_{12}^2$ term, of dimension two, which softly violates the $Z_2$ symmetry. Soft violation implies that $Z_2$ symmetry is broken near the mass shell, and is restored at small distances $\ll 1/M_i$, where $M_i$ are masses of Higgs particles. The $\lambda_6$ and $\lambda_7$ terms lead to hard violation of the $Z_2$ symmetry.

We classify the Higgs-Higgs states according to their value of the $Z_2$-parity: $\phi_i\phi_i$, $\phi_i\phi_i^*$, etc. will be called the $Z_2$-even states, while $\phi_1\phi_2$, $\phi_1\phi_2^*$, etc. will be called the $Z_2$-odd states.

### B. Tree-level unitarity constraints

(ii) The Higgs-Higgs scattering matrix at high enough energy at the tree level contains only *s*-wave amplitudes; it is described by the quartic part of the potential only. The *tree-level unitarity constraints* require that the eigenvalues of this scattering matrix be less than the unitarity limit. Violation of the tree-level unitarity constraints implies that the tree-level calculations are no more reliable and do not represent the physics of the model.

Since the coefficients of the scattering matrix at high enough energy are given only by parameters $\lambda_i$ of the Higgs potential, the tree-level unitarity constraints are written as limitations on parameters $\lambda_i$ (for example, in the minimal SM, with one Higgs doublet and $V = (\lambda/2)\times(\phi^\dagger\phi - v^2/2)^2$, such unitarity constraint is $\lambda < 16\pi/3$, [3]).

(iii) After electroweak symmetry breaking (EWSB) all eight components of two complex isodoublet fields are transformed into three Goldstone fields (which are transformed to longitudinal components of gauge bosons $W_L$, $Z_L$), two charged Higgs bosons $H^\pm$ and three neutral Higgs bosons $h_1$, $h_2$, $h_3$ (which might happen to have no definite *CP* parity).

A natural way for derivation of the tree-level unitarity constraints is to construct the scattering matrix for all the physical Higgs-Higgs (as well as $Z_L h_i$, $W_L W_L$, etc.) states in the tree approximation at high enough energy (where threshold effects are inessential) and diagonalize it. This very way was realized in the first derivation of such constraint in the Minimal standard model [3] and was repeated for the 2HDM in [4].

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The tree-level unitarity constraints are written for the scattering matrix as the limitations for its eigenvalues. They can be obtained in any basis related to the physical basis by a unitarity transformation. The derivation simplifies in the basis of the non−physical Higgs fields $\phi_a^\pm$, $n_a = \eta_a + i\xi_a$ [5,6]. An even simpler procedure developed below consists in using initial $\phi_1, \phi_2$ basis, taking into account the quantum numbers of the EW symmetry group and avoiding explicit work with components of doublets in calculation of the eigenvalues of the scattering matrix.

Until now, these constraints were considered only for the case with conserved or softly broken $Z_2$ symmetry and without *CP* violation, i.e. with $\lambda_6 = \lambda_7 = 0$ and real $\lambda_5$, $m_{12}^2$ [4–6]. These results were extended for the case with softly broken $Z_2$ symmetry and with CP violation in [7], see also recent work [8]. Here we consider the most general case. Our approach is easily applicable to other extended Higgs sectors discussed in literature.

## II. DERIVATION OF UNITARITY CONSTRAINTS

In the high-energy scalar-scalar scattering the total weak isospin $\vec{\sigma}$ and the total hypercharge $Y$ are conserved[1], with possible values $Y = 0, 2, -2$ and $\sigma = 0, 1$.

We develop a compact procedure to efficiently calculate the amplitudes of all the possible transitions. Note that a typical term in the potential $(\phi_a^*\phi_b)(\phi_c^*\phi_d)$ induces transitions in all possible cross-channels, like $\phi_a\phi_b^* \to \phi_c^*\phi_d$, $\phi_a\phi_d^* \to \phi_c^*\phi_b$, $\phi_a\phi_c \to \phi_b\phi_d$. In order to calculate the amplitude of the transition of an initial two-Higgs state $(\phi\phi)^{\rm in}$ to a final state $(\phi\phi)^f$, one needs to rewrite the potential in such a way as to obtain product $(\phi^*\phi^*)^{\rm in} \times (\phi\phi)^f$. The coefficient in front of this product gives the amplitude in question. In our calculations the isospinors $\phi_a$ (with $a = 1, 2$ indicating the doublet) are represented as columns, while $\phi_a^\dagger$ are rows.

*The hypercharge* $Y = 0$ *states*. The direct product $\phi_{b\beta}\phi_{a\alpha}^\dagger$ represents a $2\times 2$ matrix for every pair of $a$ and $b$. Since Pauli matrices plus unit matrix form a basis in the space of hermitian $2\times 2$ matrices, one can write[2] $\phi_{b\beta}\phi_{a\alpha}^\dagger = A_0\cdot\delta_{\beta\alpha} + \vec{A}\cdot\vec{\tau}_{\beta\alpha}$ with $A_0 = (\phi_a^\dagger\phi_b)/2$, $A_i = (\phi_a^\dagger\tau^i\phi_b)/2$. Therefore,

$$(\phi_{a\alpha}^*\phi_{b\alpha})(\phi_{c\beta}^*\phi_{d\beta}) = \frac{1}{2}\Big[(\phi_{a\alpha}^*\phi_{d\alpha})(\phi_{c\beta}^*\phi_{b\beta}) + \sum_r(\phi_{a\alpha}^*\tau_{\alpha\beta}^r\phi_{d\beta})(\phi_{c\gamma}^*\tau_{\gamma\delta}^r\phi_{b\delta})\Big]. \tag{3}$$

The total set of possible initial states with hypercharge $Y = 0$ in our case can be written as scalar products

$$\begin{array}{llcccc} & & \multicolumn{2}{c}{\overbrace{\qquad\qquad}^{Z_2\ \text{even}}} & \multicolumn{2}{c}{\overbrace{\qquad\qquad}^{Z_2\ \text{odd}}} \\ Y=0, & \sigma=0: & \frac{1}{\sqrt{2}}(\phi_1^\dagger\phi_1), & \frac{1}{\sqrt{2}}(\phi_2^\dagger\phi_2), & \frac{1}{\sqrt{2}}(\phi_1^\dagger\phi_2), & \frac{1}{\sqrt{2}}(\phi_2^\dagger\phi_1), \\ Y=0, & \sigma=1: & \frac{1}{\sqrt{2}}(\phi_1^\dagger\tau^i\phi_1), & \frac{1}{\sqrt{2}}(\phi_2^\dagger\tau^i\phi_2), & \frac{1}{\sqrt{2}}(\phi_1^\dagger\tau^i\phi_2), & \frac{1}{\sqrt{2}}(\phi_2^\dagger\tau^i\phi_1). \end{array} \tag{4}$$

where $i = +, z, -$.

To repeat this trick for *the hypercharge* $Y = 2$ *states*, we introduce rows $\tilde{\phi}_a = (i\tau_2\phi_a)^T = (n_a, -\phi_a^+)$ and corresponding columns $\tilde{\phi}_a^\dagger = (i\tau_2\phi_a)^*$. Note that the isoscalar form $\tilde{\phi}_{a\alpha}\phi_{b\alpha}$ is antisymmetric under permutation $a \leftrightarrow b$, $\tilde{\phi}_{a\alpha}\phi_{b\alpha} = -\tilde{\phi}_{b\alpha}\phi_{a\alpha}$, while isovector is symmetric under this permutation.

The total set of possible initial states with hypercharge $Y = 2$ can be written similarly to (4) as

$$\begin{array}{llcc} & & \overbrace{\qquad\qquad}^{Z_2\ \text{even}} & \overbrace{\qquad\qquad}^{Z_2\ \text{odd}} \\ Y=2, & \sigma=0: & \text{absent}, & \frac{1}{\sqrt{2}}(\tilde{\phi}_1\phi_2) = -\frac{1}{\sqrt{2}}(\tilde{\phi}_2\phi_1), \\ Y=2, & \sigma=1: & \frac{1}{2}(\tilde{\phi}_1\tau^i\phi_1),\quad \frac{1}{2}(\tilde{\phi}_2\tau^i\phi_2), & \frac{1}{\sqrt{2}}(\tilde{\phi}_1\tau^i\phi_2) = \frac{1}{\sqrt{2}}(\tilde{\phi}_2\tau^i\phi_1). \end{array} \tag{5}$$

The factor $1/2$ for $Z_2$-even case here is due to the presence of identical particles in the initial state. The $Z_2$ even states with $Y = 2$, $\sigma = 0$ are absent (it follows directly from the Bose-Einstein symmetry of identical scalars.). The states with $Y = -2$, $\sigma = 1$ are obtained from those for $Y = 2$ by charge conjugation.

Now similarly to (3) one can write following relation:

$$(\phi_{a\alpha}^*\phi_{b\alpha})(\phi_{c\beta}^*\phi_{d\beta}) = \frac{1}{2}\Big[(\phi_{a\alpha}^*\tilde{\phi}_{c\alpha}^*)(\tilde{\phi}_{d\beta}\phi_{b\beta}) + \sum_r(\phi_{a\alpha}^*\tau_{\alpha\beta}^r\tilde{\phi}_{c\beta}^*)(\tilde{\phi}_{d\gamma}\tau_{\gamma\delta}^r\phi_{b\delta})\Big]. \tag{6}$$

[1]This classification looks more *natural* than both the $O(4)$-classification introduced in [3] (in the minimal SM) and the scheme based on new quantum numbers $C$, $G$, and $Y_\pi$ introduced in [6].

[2]The first term $A_0$ represents isoscalar, while the second $\vec{A}$ – isovector.

For each set of states with given quantum numbers $Y$ and $\sigma$ (4) and (5), the scattering matrix in the tree approximation

$$S_{Y,\sigma} = \langle(\phi\phi)^f_{Y,\sigma}|\hat{S}|(\phi\phi)^{in}_{Y,\sigma}\rangle \tag{7}$$

is calculated easily from the potential (1) according to the procedure described above with the aid of Eqs. (3) and (6). The results are presented in (8). In each case left upper corner presents scattering matrix for $Z_2$-even states and right-down corner—for $Z_2$–odd states, while coefficients $\lambda_6$, $\lambda_7$ describe mixing among these states.

$$16\pi S_{Y=2,\sigma=1} = \begin{pmatrix} \lambda_1 & \lambda_5 & \sqrt{2}\lambda_6 \\ \lambda_5^* & \lambda_2 & \sqrt{2}\lambda_7^* \\ \sqrt{2}\lambda_6^* & \sqrt{2}\lambda_7 & \lambda_3+\lambda_4 \end{pmatrix}, \tag{8a}$$

$$16\pi S_{Y=2,\sigma=0} = \lambda_3 - \lambda_4, \tag{8b}$$

$$16\pi S_{Y=0,\sigma=1} = \begin{pmatrix} \lambda_1 & \lambda_4 & \lambda_6 & \lambda_6^* \\ \lambda_4 & \lambda_2 & \lambda_7 & \lambda_7^* \\ \lambda_6^* & \lambda_7^* & \lambda_3 & \lambda_5^* \\ \lambda_6 & \lambda_7 & \lambda_5 & \lambda_3 \end{pmatrix}, \tag{8c}$$

$$16\pi S_{Y=0,\sigma=0} = \begin{pmatrix} 3\lambda_1 & 2\lambda_3+\lambda_4 & 3\lambda_6 & 3\lambda_6^* \\ 2\lambda_3+\lambda_4 & 3\lambda_2 & 3\lambda_7 & 3\lambda_7^* \\ 3\lambda_6^* & 3\lambda_7^* & \lambda_3+2\lambda_4 & 3\lambda_5^* \\ 3\lambda_6 & 3\lambda_7 & 3\lambda_5 & \lambda_3+2\lambda_4 \end{pmatrix}. \tag{8d}$$

The unitarity constraint means that $S < 1$, therefore it limits the eigenvalues of the written matrices $\Lambda$ by inequalities

$$|\Lambda| < 16\pi. \tag{9}$$

Unfortunately, explicit expressions for these eigenvalues are very complex since they should be obtained from equations of the 3rd or 4th degree.

However it is useful to present a result for the case of softly broken $Z_2$ symmetry with possible $CP$ violation (obtained in [7] as generalization of [5]). In this case $\lambda_6 = \lambda_7 = 0$, our scattering matrices become block diagonal and their eigenvalues are calculated easily. Now all eigenvalues of above scattering matrices can be written as $\Lambda^{Z_2}_{Y\sigma\pm}$

$$\begin{aligned}
\Lambda^{\text{even}}_{21\pm} &= \frac{1}{2}\left(\lambda_1+\lambda_2 \pm \sqrt{(\lambda_1-\lambda_2)^2+4|\lambda_5|^2}\right),\\
\Lambda^{\text{odd}}_{21} &= \lambda_3+\lambda_4, \qquad \Lambda^{\text{odd}}_{20} = \lambda_3-\lambda_4,\\
\Lambda^{\text{even}}_{01\pm} &= \frac{1}{2}\left(\lambda_1+\lambda_2 \pm \sqrt{(\lambda_1-\lambda_2)^2+4\lambda_4^2}\right),\\
\Lambda^{\text{odd}}_{01\pm} &= \lambda_3 \pm |\lambda_5|,\\
\Lambda^{\text{even}}_{00\pm} &= \frac{1}{2}\left[3(\lambda_1+\lambda_2) \pm \sqrt{9(\lambda_1-\lambda_2)^2+4(2\lambda_3+\lambda_4)^2}\right],\\
\Lambda^{\text{odd}}_{00\pm} &= \lambda_3+2\lambda_4 \pm 3|\lambda_5|.
\end{aligned} \tag{10}$$

The obtained constraints (9) and (10) differ from those obtained in Ref. [5] only by the change $\lambda_5 \to |\lambda_5|$.

(iv) To describe the general case with hard violation of $Z_2$ symmetry, we use following fact:

For a Hermitian matrix $\mathcal{M} = ||M_{ij}||$ with maximal and minimal eigenvalues $\Lambda_+$ and $\Lambda_-$, respectively, all diagonal matrix elements $M_{ii}$ lie between these eigenvalues,

$$\Lambda_+ \geq M_{ii} \geq \Lambda_-. \tag{11}$$

This fact follows from extremal properties of the $n$-dimensional ellipsoid, that is $\Lambda_- \sum x_i^2 \leq \sum M_{ij}x_ix_j \leq \Lambda_+ \sum x_i^2$. (For $2\times 2$ matrix proof is evident.)

The diagonalization of scattering matrices, yielding their eigenvalues, can be realized in two steps. First, we can diagonalize corners of these matrices corresponding to fixed values of the $Z_2$ parity. At this step we obtain scattering matrices with diagonal elements described by Eqs. (10). Therefore, by virtue of (11) the constraints (9) and (10) are *necessary* conditions for unitarity. They are enhanced due to $\lambda_6$, $\lambda_7$ terms describing hard violation of the $Z_2$ symmetry. The shift of eigenvalues (10) caused by these terms can be easily calculated in the case of a weak hard violation of $Z_2$ symmetry[3] $|\lambda_{6,7}| \ll \Lambda^{Z_2}_{Y,\sigma}$.

## III. DISCUSSION AND COMMENTS

### A. Some invariants of reparametrization transformations

The 2HDM contains two doublet fields, $\phi_1$ and $\phi_2$, with identical quantum numbers. Therefore, its most general

[3] In our opinion, precise equations for eigenvalues with solutions of equations of 3rd or 4th degree have no big sense.

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 (the reparametrization invariance), see for details [2].

The eigenvalues of scattering matrices (8) are—by construction—reparametrization invariant quantities. In the standard equations for eigenvalues of these matrices their coefficients are also invariants of reparametrization transformation[4] since they can be constructed from the eigenvalues. Each $n \times n$ matrix $S_{Y\sigma}$ in (8) generates $n$ invariant polynomials of $\lambda_i$: one of the first, one of the second, etc. order. A convenient choice of these invariants is $\mathrm{Tr}\{S^k_{Y\sigma}\}$ for $k = 1, \ldots, n$. ($\mathrm{Det}\{S_{Y\sigma}\}$ can be also used instead of $\mathrm{Tr}\{S^n_{Y\sigma}\}$.) It gives 12 invariants. Of course, not all of them are independent. For example, among the four invariants linear in $\lambda_i$, which we denote $I_{Y\sigma} \equiv 16\pi \mathrm{Tr}\{S_{Y\sigma}\}$ according to their $Y$ and $\sigma$,

$$I_{21} = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4, \qquad I_{20} = \lambda_3 - \lambda_4,$$
$$I_{01} = \lambda_1 + \lambda_2 + 2\lambda_3, \qquad I_{00} = 3(\lambda_1 + \lambda_2) + 2\lambda_3 + 4\lambda_4 \tag{12}$$

only two are linearly independent. This is related to the fact that there exist only two independent linear combination of parameters $\lambda_i$ of the general quartic 2HDM potential, corresponding to two scalars of the $SU(2) \times U(1)$ group, describing reparametrization symmetry [10]. We checked that all $Tr\{S^k_{Y\sigma}\}$ can be expressed in terms of invariants derived in [10]. This argument can be inverted, namely, there exists a subset $\{I_i\}$, $i = 1, \ldots 7$ of all traces of scattering matrices such that all 7 invariants of [10] can be expressed via members of $\{I_i\}$. This means that in the general 2HDM there are at most 7 independent tree-level unitarity constraints.

### B. Limitations for masses

In early works, e.g. [4], where some restricted versions of the 2HDM were considered, the unitarity constraints in 2HDM were presented as constraints on masses of all the physical Higgs bosons. In the most general 2HDM such a direct link between the two sets of constraints is lost. In the tree approximation considered here the masses of Higgs bosons are composed from quantities $\lambda_i$, vacuum expectation values of Higgs fields $v_1, v_2$ and quantity $\nu \propto Re(\overline{m}^2_{12})/v_1 v_2$ (the quantity $m^2_{12}$ in a special rephasing gauge, which can be different from that used above, see [2] for details). Since parameter $m^2_{12}$ does not enter the quartic interactions, the above unitarity constraints, generally, do not set upper bounds for the masses of *all* the observable Higgs bosons, which was explicitly noted in [6]. Reasonable limitations on these masses can be obtained for some specific values of $\nu$. For example, for reasonably small value of $\nu$ one can have the lightest Higgs boson mass of about 120 GeV and the masses of other Higgs bosons can be up to about 600 GeV without violation of tree-level unitarity [2]. At large $\nu$, masses of all Higgs bosons except the lightest one can be very large without violation of unitarity constraint.

### C. Unitarity constraints and strong interaction in Higgs sector

Let us discuss briefly some new features, which are brought up by the situation with unitarity constraints in 2HDM.

The unitarity constraints were obtained first [3] in the minimal SM. In this model, the Higgs boson mass $M_H = v\sqrt{\lambda}$, and its width $\Gamma$ (given mainly by decay to longitudinal components of gauge bosons $W_L$, $Z_L$) grows as $\Gamma \propto M^3_H$. The unitarity limit corresponds to the case when $\Gamma_H \approx M_H$, so that the physical Higgs boson disappears, the strong interaction in the Higgs sector is realized as strong interaction of longitudinal components of gauge bosons $W_L$, $Z_L$ at $\sqrt{s} > v\sqrt{\lambda} \gtrsim v\sqrt{16\pi/3} \approx 1$ TeV. Therefore, if $\lambda$ exceeds the tree-level unitarity limitation, the discussion in terms of observable Higgs particle becomes meaningless, and a new physical picture for the Electroweak Symmetry Breaking in SM arises.

Such type of correspondence among the tree-level unitarity limit, realization of the Higgs field as more or less narrow resonance and a possible strong $W_L W_L$ and $Z_L Z_L$ interaction, can generally be violated in the 2HDM if values of $\lambda_i$ differ from each other essentially. Large number of degrees of freedom of 2HDM generates situations when some of Higgs bosons of this theory are "normal" more or less narrow scalars (whose properties can be estimated perturbatively), while the other scalars and (or) $W_L$, $Z_L$ interact strongly at sufficiently high energy. It can happen that some of the latter can be realized as physical particles, while the other disappear from particle spectrum like Higgs boson in SM with large $\lambda$. In such cases the unitarity constraints work in different way for different *physical* channels. The list of possibilities will be studied elsewhere.

## IV. CONCLUSIONS

We derived the tree-level unitarity constraints in the most general 2HDM with explicit $CP$-violation. A significant point of work is a natural self-suggesting classification of two-Higgs states and a compact representation of the Higgs-Higgs scattering matrix at high energies. We discussed the link between these constraints and limitations of masses of the physical Higgs bosons, as well as the possibility of strong interaction in the Higgs sector.

The scheme we proposed can be readily exploited in the study of some other multi-Higgs models. For example, the

[4]This set of invariants presents important subset from huge set considered in Ref. [9].

model with *two Higgs doublets plus one Higgs singlet* *($\sigma = 0$) with* $Y = 0$ can be described by potential (1) plus additional terms. In this case scattering matrices $S_{Y=2,\sigma}$, $S_{Y=0,\sigma=1}$ have the form (8a)–(8c) while scattering matrix $S_{Y=0,\sigma=0}$ is obtained from that written in (8d) by adding of one column and one row. Besides, only one new scattering matrix $S_{Y=1,\sigma=1/2}$ appears in this case.

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