

# BSMPT v2

## A Tool for the Electroweak Phase Transition and the Baryon Asymmetry of the Universe in Extended Higgs Sectors

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### Abstract

We present the C++ code **BSMPT v2** which is an extension of the previous code **BSMPT** for the calculation of the strength of the electroweak phase transition in extended Higgs sectors. The new version **BSMPT v2** includes the features of **BSMPT** and extends the already implemented models (the 2-Higgs-Doublet model (2HDM) in its CP-conserving and CP-violating versions and the Next-to-2HDM) by the Complex Singlet Extension of the Standard Model (CxSM). The major upgrade is the implementation of the computation of the baryon asymmetry of the Universe for the CP-violating 2HDM (C2HDM), which is performed in two different approximations. These changes and further smaller modifications are described in this manual. Additionally, a detailed explanation of the procedure for the implementation of new models is given, which has also changed with respect to the previous version.

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# Program Summary

**Program Title:** BSMPT

**Licensing provisions:** GPL-3.0 License

**Programming Language:** C++14

**Nature of problem:** Non-minimal extended Higgs sector models provide non-trivial vacuum structures which allow for a strong first order electroweak phase transition. Such a phase transition is one of the three Sakharov conditions that are required for a dynamical generation of the observed baryon asymmetry of the universe (BAU) through an electroweak phase transition. The actual calculation of the electroweak baryogenesis requires the solution of the quantum transport equation system describing the non-thermal equilibrium state of the early universe during the phase transition. BSMPT v2 provides a numerical tool to investigate the vacuum structure of the one-loop effective potential at finite temperature including thermal masses, for an arbitrary extended Higgs sector. It allows for the computation of the strength of the electroweak phase transition for the implemented models. For the CP-violating 2HDM (C2HDM) also the generated BAU is calculated. For the latter task BSMPT v2 has two different approaches implemented for the formulation of the quantum transport equations, given by the FH approach based on the semi-classical force and the vacuum expectation value insertion method VIA.

**Solution Method:** Numerical minimization of the one-loop effective potential including thermal masses, at finite temperature with three different numerical minimizers, `GSL`, `cmaes` and `NLopt`, in order to determine the relevant parameters required for the phase transition dynamics at the critical temperature and the critical field configuration. Furthermore, with the updated version BSMPT v2 it is possible to numerically solve for the C2HDM the system of coupled differential transport equations and calculate the BAU for this model.

**Additional comments including restrictions and unusual features:** The BSM extensions are restricted to the Higgs sectors. New gauge bosons and fermions would require an adaption in the thermal corrections of the one-loop potential, which is not implemented in BSMPT v2. At present, the BAU is only calculated for the C2HDM. In the computation of the BAU the wall velocity is an input parameter and assumed to be small, for the VEV configuration a kink profile is assumed, the nucleation temperature is approximated by the critical temperature.

## 1 Introduction

One of the unsolved puzzles of particle physics is the observed baryon asymmetry of the Universe (BAU) [1]. Electroweak baryogenesis plays an important role in this context, as it provides a mechanism to generate the BAU dynamically in the early Universe through a strong first order electroweak phase transition (SFOEWPT) [2–10] provided all three Sakharov conditions [11] are fulfilled. Within the Standard Model (SM), in principle all three conditions can be fulfilled, leading, however, to a phase transition (PT) that is not of strong first order [10, 12–18]. Therefore, new physics extensions are required providing both additional sources of CP violation and further scalar states that are able to trigger an SFOEWPT. In order to answer the question if a specific model can explain the BAU based on electroweak baryogenesis, we have to investigate if the phase transition triggered by its Higgs potential is of strong first order and if the baryon asymmetry generated by the model matches the measured value of  $5.8 \cdot 10^{-10} < \eta < 6.5 \cdot 10^{-10}$  [19] quantitatively. The strength of the phase transition is defined by the quotient  $\xi_c$  of the vacuum expectation value (VEV)  $v_c$  at the critical temperature  $T_c$ , with  $T_c$ , defined as the temperature where two degenerate global minima exist. Both quantities are obtained from

the loop-corrected effective Higgs potential at finite temperature. A value of  $\xi_c = v_c/T_c > 1$  indicates an SFOEWPT [5,20]. For the actual computation of the BAU it is required to describe the thermal system of the early universe. The latter requires the knowledge of the chemical potentials of all contributing particles in front of the bubble wall which in turn are obtained from the solution of the (quantum) transport equations.

In the following we present version 2 of the C++ code BSMPT (Beyond the Standard Model Phase Transitions) [21].<sup>1</sup> It extends the previous code for the computation of the phase transition by the calculation of the BAU or the CP-violating 2-Higgs-Doublet Model (C2HDM). In detail, BSMPT v2 includes the features of the previous version, that are:

- \* Calculation of  $v_c$ ,  $T_c$  and  $\xi_c$  from the loop-corrected effective potential at finite temperature [25–27] including the daisy resummation for the bosonic masses [28]. Two different approximations for the treatment of the thermal masses are implemented, the Parwani [29] and the Arnold-Espinosa method [30] with the latter set by default. The renormalisation of the potential is based on physical 'on-shell' conditions in the sense that the loop-corrected masses and mixing angles extracted from the effective potential are equal to their tree-level input values [31].
- \* Calculation of the evolution of the VEVs as a function of the temperature.
- \* Calculation of the global minimum of the one-loop corrected potential at zero temperature.
- \* Calculation of the loop-corrected trilinear Higgs self-couplings in the on-shell scheme defined in [31].

The first BSMPT version includes as predefined models the CP-conserving 2-Higgs-Doublet Model (2HDM) [32,33] and its CP-violating version, the C2HDM [34–37], as well as the Next-to-2HDM (N2HDM) [38–40]. For applications of BSMPT to phenomenological investigations of these models, see [31, 41, 42].

The newly implemented features in BSMPT v2, which will be presented in this paper, are

- \* The computation of the BAU for the C2HDM. It is performed in two different approximations, the first approach is based on the semi-classical force [43–46] yielding a set of fluid equations, which we refer to as FH approach. The second approach is based on the VEV insertion approximation (VIA) method [47, 48]. The implementation of the accordingly adapted transport equations in the latter approach follows [49]. Since both approaches rely on the same assumption on the wall profile, BSMPT v2 allows for their comparison and discussion. The implemented wall profile is approximated by the Kink profile [44, 79]. A systematic comparison of the various approximations and their impact on non-minimal models has not been available so far. Our code therefore offers deliberately to the user the option to choose among various approximations to study their impact and get a feeling for the validity of the applied approximations.

Note that at present in the FH approach we assume small values for the wall velocity, which is an additional input parameter. Therefore, wall velocities with values close to the plasma speed should be taken with caution. An extension to arbitrary wall velocities as provided recently in [50] is left for future work. In the FH approach, we also implemented a second variant of the transport equations using plasma velocities expressed through derivatives.

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<sup>1</sup>Further public codes for the analysis of the possible phases and phase transitions in the early Universe are CosmoTransitions [22], PhaseTracer [23] and BubbleProfiler [24]

So far, the computation of the BAU can be performed only for the C2HDM. Extensions to other models are planned for future versions of the code.

- \* Implementation of a new model, the Complex Singlet Extension of the SM (CxSM).

Further differences of BSMPT v2 with respect to the first BSMPT version are

- \* BSMPT can now be exported as library.
- \* The interfaces of the various functions have changed.
- \* The code base has been improved and changed from C++11 to C++14.

In this paper, we present the new features of BSMPT v2, which can be downloaded at:

<https://github.com/phbasler/BSMPT>

We start by reviewing in Sec. 2 the newly implemented SM extension by a complex singlet field, the CxSM. In Sec. 3, the implementation of the calculation of the BAU for the C2HDM is presented in detail. In Sec. 3.1 the applied treatment of the wall profile is discussed before presenting in Sec. 3.2 the FH approach and in Sec. 3.3 the VIA approach for the calculation of the BAU. Sec. 4 is devoted to the program description, specifying the system requirements, the installation and usage of the program. For completeness, we repeat the features of the first version of BSMPT when presenting the new modules and functions of BSMPT v2. In the computation of the baryon asymmetry we apply a number of approximations. While a systematic comparison of the various approximations and their impact on non-minimal models has not been available so far, our code has been set up such that the user has the option to choose among various approximations which allows for the study of their impact. In Sec. 5, we present a generic discussion of the approximations and options that are provided in order to give some guidance to the user. The code allows for the implementation of a new model by the user. Since this feature has changed in BSMPT v2 with respect to the original version of the code, Sec. 6 explains in detail, with the help of a toy model, the steps necessary to implement a new model in BSMPT v2. Previously implemented models by the user will have to be adapted to the new procedure in order to use BSMPT v2. Sec. 7 comments on the usage of BSMPT as library and Sec. 8 on the upgrade from v1 to v2. We conclude in Sec. 9.

The version BSMPT v2 presented in this paper can be understood as a first proof of concept for combining our computation of the electroweak phase transition using on-shell renormalisation with the calculation of the BAU in two different approaches. The code will continuously be updated in future to implement extensions of the approximations used here and to extend it to new models. The paper will be accompanied by a forthcoming paper [51] applying the computation of the BAU to a specific model including the up-to-date theoretical and experimental constraints.

## 2 The Newly Implemented Model CxSM

The new version of BSMPT has been extended to include an additional model, the Complex Singlet Extension of the SM (CxSM) [52–60]. Since the general calculation of the one-loop effective potential at finite temperature does not differ from the previous version of BSMPT, we skip the introduction of the effective potential and refer to [21] for details, for specific model

discussions we refer to [31, 41, 42]. The Higgs potential of the CxSM is based on the extension of the SM Higgs potential by a complex scalar singlet field  $\mathbb{S}$ . The tree-level potential with a softly broken global  $U(1)$  symmetry is given by

$$V = \frac{m^2}{2} \Phi^\dagger \Phi + \frac{\lambda}{4} (\Phi^\dagger \Phi)^2 + \frac{\delta_2}{2} \Phi^\dagger \Phi |\mathbb{S}|^2 + \frac{b_2}{2} |\mathbb{S}|^2 + \frac{d_2}{4} |\mathbb{S}|^4 + \left( \frac{b_1}{4} \mathbb{S}^2 + a_1 \mathbb{S} + c.c. \right), \quad (1)$$

where

$$\mathbb{S} = \frac{1}{\sqrt{2}} (S + iA) \quad (2)$$

is a hypercharge zero scalar field. The soft-breaking terms are written in parenthesis. After electroweak symmetry breaking the Higgs doublet field  $\Phi$  and the singlet field  $\mathbb{S}$  can be written as

$$\Phi = \frac{1}{\sqrt{2}} \begin{pmatrix} G^+ \\ v + h + iG^0 \end{pmatrix}, \quad (3)$$

$$\mathbb{S} = \frac{1}{\sqrt{2}} (s + v_s + i(a + v_a)), \quad (4)$$

where  $v \approx 246$  GeV is the SM vacuum expectation value (VEV) of  $h$  and  $v_s$  and  $v_a$  are the VEVs of the real and imaginary parts of the complex singlet field, respectively. Because of the hermicity of the potential, all parameters in Eq. (1) are real, except for  $b_1$  and  $a_1$ . The complex phases can be reabsorbed through a redefinition of the fields so that either the phase of  $b_1$  or  $a_1$  can be set to zero. The user can choose among the two options that have both been implemented in BSMPT.

The mass eigenstates  $h_i$  ( $i = 1, 2, 3$ ) are obtained from the gauge fields  $h, s, a$  in Eqs. (3), (4) through a rotation

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R \begin{pmatrix} h \\ s \\ a \end{pmatrix}, \quad (5)$$

with ( $\mathcal{M}^2$  denotes the mass matrix squared in the gauge basis)

$$R \mathcal{M}^2 R^T = \text{diag}(m_{h_1}^2, m_{h_2}^2, m_{h_3}^2) \quad (6)$$

and  $m_{h_1} \leq m_{h_2} \leq m_{h_3}$  by convention. The  $3 \times 3$  rotation matrix is parametrised in terms of three mixing angles  $\alpha_i$  ( $i = 1, 2, 3$ )

$$R = \begin{pmatrix} c_1 c_2 & s_1 c_2 & s_2 \\ -(c_1 s_2 s_3 + s_1 c_3) & c_1 c_3 - s_1 s_2 s_3 & c_2 s_3 \\ -c_1 s_2 c_3 + s_1 s_3 & -(c_1 s_3 + s_1 s_2 c_3) & c_2 c_3 \end{pmatrix}, \quad (7)$$

where the shorthand notation  $c_i \equiv \cos \alpha_i$  and  $s_i \equiv \sin \alpha_i$  has been introduced. Without loss of generality, the interval of the mixing angles is taken as

$$-\pi/2 \leq \alpha_i < \pi/2. \quad (8)$$

The minimum conditions of the potential

$$0 = v \left( \frac{\lambda}{4} v^2 + \frac{\delta_2}{4} (v_a^2 + v_s^2) + \frac{m^2}{2} \right) \quad (9)$$

$$0 = \text{Re}(a_1) \sqrt{2} - \text{Im}(b_1) \frac{v_a}{2} + v_s \left( \frac{d_2}{4} (v_s^2 + v_a^2) + \frac{\delta_2}{4} v^2 + \frac{1}{2} \text{Re}(b_1) + \frac{1}{2} b_2 \right) \quad (10)$$

$$0 = -\text{Im}(a_1) \sqrt{2} - \text{Im}(b_1) \frac{v_s}{2} + v_a \left( \frac{d_2}{4} (v_s^2 + v_a^2) + \frac{\delta_2}{4} v^2 - \frac{1}{2} \text{Re}(b_1) + \frac{b_2}{2} \right) \quad (11)$$

are used to express the parameters of the potential in terms of the input parameters. These depend on the choice of the VEV configuration of the singlet field, *cf.* App. A.

The counterterm potential of the CxSM reads

$$\begin{aligned} V^{\text{CT}} = & \frac{\delta m^2}{2} \Phi^\dagger \Phi + \frac{\delta \lambda}{4} (\Phi^\dagger \Phi)^2 + \frac{\delta \delta_2}{2} \Phi^\dagger \Phi |\mathbb{S}|^2 + \frac{\delta b_2}{2} |\mathbb{S}|^2 + \frac{\delta d_2}{4} |\mathbb{S}|^4 \\ & + \left( \frac{1}{2} \delta \text{Re}(b_1) ((\text{Re}\mathbb{S})^2 - (\text{Im}\mathbb{S})^2) - \text{Re}\mathbb{S} \text{Im}\mathbb{S} \delta \text{Im} b_1 + 2\delta a_1 \text{Re}\mathbb{S} - 2\delta a_1 \text{Im}\mathbb{S} \right) \\ & + \delta T_h (h + \omega_h) + \delta T_s (s + \omega_s) + \delta T_a (a + \omega_a) , \end{aligned} \quad (12)$$

with the tadpole counterterms  $\delta T_i$  for each field with a non-zero VEV. We use the symbol  $\omega$  to generically denote VEVs including loop and non-zero temperature effects in the potential. The renormalisation conditions presented in [21, 31, 41, 42] allow to use the loop-corrected masses and mixing angles as direct inputs of the parameter scan since these conditions require the loop-corrected masses derived from the effective potential to be equal to their tree-level values. In this sense we call them 'on-shell' although this expression should be taken with caution here, since the loop-corrected masses extracted from the effective potential are evaluated at vanishing external momentum, whereas on-shell conditions in the proper sense demand the renormalised mass to be equal to the tree-level one at momentum squared equal to the mass squared of the particle. While the zero-momentum approximation used in the 'on-shell' definition deteriorates with rising particle mass the loop corrections to heavy particles are in general small<sup>2</sup> on the other hand. Therefore, we expect the impact of the missing pieces to be small.

In the following we list the counterterms for the various possible VEV configurations, where we use the shorthand notations

$$N_{\phi_i}^{\text{CW}} = \frac{\partial V^{\text{CW}}}{\partial \phi_i}, \quad H_{\phi_i, \phi_j}^{\text{CW}} = \frac{\partial^2 V^{\text{CW}}}{\partial \phi_i \partial \phi_j}, \quad (13)$$

for the first and second derivatives of the Coleman-Weinberg potential. The parameters  $t_i \in \mathbb{R}$  ( $i = 1, 2, 3, 4$ ) that appear in the following counterterms can be chosen freely. For simplicity, in the implementation in BSMPT, they are set to zero.

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<sup>2</sup>See for example Ref. [61] for an overview of the computation of mass corrections in the effective potential approach and explicit diagrammatic calculations in supersymmetric models.

Case  $v_a \neq 0$  and  $v_s \neq 0$ :

$$\delta\lambda = \frac{2}{v^2} (H_{G_0, G_0}^{\text{CW}} - H_{h, h}^{\text{CW}}) \quad (14a)$$

$$\delta m^2 = \frac{v_a}{v} H_{h, a}^{\text{CW}} - 3H_{G_0, G_0}^{\text{CW}} + H_{h, h}^{\text{CW}} + \frac{v_s^2}{vv_a} H_{h, a}^{\text{CW}} \quad (14b)$$

$$\delta\delta_2 = -\frac{2}{v_a v} H_{h, a}^{\text{CW}} \quad (14c)$$

$$\delta b_2 = H_{h, a}^{\text{CW}} \frac{v}{v_a} - H_{s, s}^{\text{CW}} + 2\frac{v_a}{v_s} H_{s, a}^{\text{CW}} - H_{a, a}^{\text{CW}} - t_1 \left( \frac{v_a}{v_s} + \frac{v_s}{v_a} \right) \quad (14d)$$

$$\delta d_2 = -\frac{2}{v_a v_s} H_{s, a}^{\text{CW}} + \frac{t_1}{v_a v_s} \quad (14e)$$

$$\delta \text{Re} b_1 = H_{a, a}^{\text{CW}} - H_{s, s}^{\text{CW}} + H_{s, a}^{\text{CW}} \left( \frac{v_s}{v_a} - \frac{v_a}{v_s} \right) + t_1 \left( \frac{v_a}{2v_s} - \frac{v_s}{2v_a} \right) \quad (14f)$$

$$\delta \text{Im} b_1 = t_1 \quad (14g)$$

$$\delta \text{Re} a_1 = \frac{1}{\sqrt{2}} \left( H_{s, s}^{\text{CW}} v_s - H_{s, a}^{\text{CW}} \frac{v_s^2}{v_a} - N_s^{\text{CW}} \right) - \frac{1}{\sqrt{2}} t_2 + \frac{\sqrt{2}}{4} t_1 \left( v_a + \frac{v_s^2}{v_a} \right) \quad (14h)$$

$$\delta \text{Im} a_1 = \frac{1}{\sqrt{2}} \left( H_{s, a}^{\text{CW}} \frac{v_a^2}{v_s} - H_{a, a}^{\text{CW}} v_a + N_a^{\text{CW}} \right) + \frac{1}{\sqrt{2}} t_3 - \frac{\sqrt{2}}{4} t_1 \left( \frac{v_a^2}{v_s} + v_s \right) \quad (14i)$$

$$\delta T_h = H_{G_0, G_0}^{\text{CW}} v - N_h^{\text{CW}} \quad (14j)$$

$$\delta T_s = t_2 \quad (14k)$$

$$\delta T_a = t_3. \quad (14l)$$

Case  $v_s \neq 0$  and  $v_a = 0$ :

$$\delta m^2 = H_{h, h}^{\text{CW}} - 3H_{G_0, G_0}^{\text{CW}} + \frac{v_s}{v} H_{h, s}^{\text{CW}} \quad (15a)$$

$$\delta\lambda = \frac{2}{v^2} (H_{G_0, G_0}^{\text{CW}} - H_{h, h}^{\text{CW}}) \quad (15b)$$

$$\delta\delta_2 = -\frac{2}{vv_s} H_{h, s}^{\text{CW}} \quad (15c)$$

$$\delta b_2 = H_{s, s}^{\text{CW}} - H_{a, a}^{\text{CW}} + \frac{v}{v_s} H_{h, s}^{\text{CW}} - \frac{2}{v_s} N_s^{\text{CW}} - \frac{2\sqrt{2}}{v_s} t_1 - \frac{2}{v_s} t_2 \quad (15d)$$

$$\delta d_2 = \frac{1}{v_s^3} \left( -2H_{s, s}^{\text{CW}} v_s + 2\sqrt{2} t_1 + 2N_s^{\text{CW}} + 2t_2 \right) \quad (15e)$$

$$\delta \text{Re} b_1 = H_{a, a}^{\text{CW}} - \frac{\sqrt{2}}{v_s} t_1 + \frac{1}{v_s} N_s^{\text{CW}} - \frac{t_2}{v_s} \quad (15f)$$

$$\delta \text{Im} b_1 = 2H_{s, a}^{\text{CW}} \quad (15g)$$

$$\delta \text{Re} a_1 = t_1 \quad (15h)$$

$$\delta \text{Im} a_1 = \frac{1}{\sqrt{2}} (t_3 + N_a^{\text{CW}} - H_{s, a}^{\text{CW}} v_s) \quad (15i)$$

$$\delta T_h = H_{G_0, G_0}^{\text{CW}} v - N_h^{\text{CW}} \quad (15j)$$

$$\delta T_s = t_2 \quad (15k)$$

$$\delta T_a = t_3. \quad (15l)$$

Case  $v_a \neq 0$  and  $v_s = 0$ :

$$\delta m^2 = H_{h,h}^{\text{CW}} - 3H_{G_0,G_0}^{\text{CW}} + \frac{v_a}{v} H_{h,a}^{\text{CW}} \quad (16a)$$

$$\delta \lambda = \frac{2}{v^2} (H_{G_0,G_0}^{\text{CW}} - H_{h,h}^{\text{CW}}) \quad (16b)$$

$$\delta \delta_2 = -\frac{2}{vv_a} H_{h,a}^{\text{CW}} \quad (16c)$$

$$\delta b_2 = \frac{2\sqrt{2}}{v_a} t_1 - \frac{2}{v_a} t_3 H_{a,a}^{\text{CW}} - H_{s,s}^{\text{CW}} + \frac{v}{v_a} H_{h,a}^{\text{CW}} - \frac{2}{v_a} N_a^{\text{CW}} \quad (16d)$$

$$\delta d_2 = \frac{2}{v_a^3} (t_3 - \sqrt{2}t_1) + \frac{2N_a^{\text{CW}} - 2H_{a,a}^{\text{CW}}v_a}{v_a^3} \quad (16e)$$

$$\delta \text{Re}b_1 = \frac{t_3 - \sqrt{2}t_1}{v_a} + \frac{N_a^{\text{CW}}}{v_a} - H_{s,s}^{\text{CW}} \quad (16f)$$

$$\delta \text{Im}b_1 = 2H_{s,a}^{\text{CW}} \quad (16g)$$

$$\delta \text{Re}a_1 = -\frac{1}{\sqrt{2}} (t_2 + N_s^{\text{CW}} - H_{s,a}^{\text{CW}}v_a) \quad (16h)$$

$$\delta \text{Im}a_1 = t_1 \quad (16i)$$

$$\delta T_h = H_{G_0,G_0}^{\text{CW}}v - N_h^{\text{CW}} \quad (16j)$$

$$\delta T_s = t_2 \quad (16k)$$

$$\delta T_a = t_3. \quad (16l)$$

Case  $v_a = v_s = 0$ :

$$\delta m^2 = H_{h,h}^{\text{CW}} - 3H_{G_0,G_0}^{\text{CW}} \quad (17a)$$

$$\delta \lambda = \frac{2}{v^2} (H_{G_0,G_0}^{\text{CW}} - H_{h,h}^{\text{CW}}) \quad (17b)$$

$$\delta \delta_2 = t_1 \quad (17c)$$

$$\delta b_2 = -\frac{v^2}{2} t_1 - H_{s,s}^{\text{CW}} - H_{a,a}^{\text{CW}} \quad (17d)$$

$$\delta d_2 = t_2 \quad (17e)$$

$$\delta \text{Re}b_1 = H_{a,a}^{\text{CW}} - H_{s,s}^{\text{CW}} \quad (17f)$$

$$\delta \text{Im}b_1 = 2H_{s,a}^{\text{CW}} \quad (17g)$$

$$\delta \text{Re}a_1 = -\frac{1}{\sqrt{2}} (t_3 + N_s^{\text{CW}}) \quad (17h)$$

$$\delta \text{Im}a_1 = \frac{1}{\sqrt{2}} (t_4 + N_a^{\text{CW}}) \quad (17i)$$

$$\delta T_h = H_{G_0,G_0}^{\text{CW}}v - N_h^{\text{CW}} \quad (17j)$$

$$\delta T_s = t_3 \quad (17k)$$

$$\delta T_a = t_4. \quad (17l)$$

Note that we treat the complex singlet field with respect to the minimisation in all cases in the same way regardless of the VEV configuration, meaning that the singlet fields  $s, a$  in Eq. (4) are allowed to evolve a non-zero VEV at finite temperature even when the zero temperature values

are chosen to be zero. In this way it is possible to investigate the stability of the Dark Matter candidate at non-zero temperatures.

### 3 Calculation of the Baryon Asymmetry of the Universe

In this section we will briefly document the approaches implemented in `BSMPT v2` used for the calculation of BAU. So far, two non-local approaches are implemented. These are the semi-classical force approach [43–46], based on a WKB approximation of the (quantum) transport equations, and the competing VEV-insertion approach [47, 48]. Both of them rely on the same assumptions concerning the wall profile, so that the results provided by `BSMPT` for the two different implementations allow for their comparison and discussion. We will start by reviewing the calculation of the bubble wall profile, followed by the calculation of the wall thickness. We will then list the formulas required in the two approaches for the transport equations.

#### 3.1 Wall Profile

Both approaches assume a planar bubble wall. The thus omitted curvature terms in the wall profile simplify the derivation of the transport equations significantly. The dimensionality of the problem reduces from  $3 + 1$  to an effective  $1 + 1$  problem, with only one space coordinate  $z$ . The space coordinate will be referred to as bubble wall distance in the following. In a first approach, the wall profile is approximated by the Kink profile [44],

$$f(z) = \frac{f_0}{2} \left( 1 - \tanh \frac{z}{L_W} \right), \quad (18)$$

where  $f_0$  indicates the value of the VEV inside the broken phase and  $L_W$  describes the wall thickness. While this is not an optimal approach, it is an approach that is frequently used in the literature. We varied the wall thickness for specific benchmark points to investigate the impact on the BAU. It turned out that the impact on the  $\eta$  value was in the percentage region. We plan to investigate the true bounce solution in future, which would allow us to estimate the true error.

The critical temperature  $T_c$  is defined by the coexistence of two degenerate minima of the potential, the broken non-zero VEV and the symmetric vanishing one. The wall thickness  $L_W$  can be related to the barrier height  $V_b$  between both minima as [44]

$$L_W = \frac{v_c}{\sqrt{8V_b}}, \quad (19)$$

with the critical VEV  $v_c$  at  $T_c$  given by the VEV of the broken minimum. In fact, the actual nucleation of the bubbles happens at the nucleation temperature  $T_N < T_c$ . Since `BSMPT v2` cannot estimate the nucleation temperature, the wall thickness and thus the bubble wall profile are determined at the critical temperature.

The calculation of the barrier height between both minima is implemented as follows: A straight line between both minima in the VEV vector space  $\{\vec{\omega}\}$  is taken as a first guess for the tunnel path, parametrised with  $t \in [0, 1]$  as

$$\Gamma : \vec{\omega}(t) = \vec{\omega}_s + t\vec{n}, \quad \text{with} \quad \vec{n} = \vec{\omega}_b - \vec{\omega}_s. \quad (20)$$

The broken VEV configuration  $\vec{\omega}_b$  is evaluated by the `BSMPT` routine. The complex phase of the symmetric VEV configuration is arbitrary due to the vanishing VEV. However, we want to

define the symmetric phase such that we have a smooth function if an infinitesimal step is taken along the tunnel path. For that reason, we determine the global minimum in the orthogonal plane

$$\vec{\omega} \in \{ \vec{x} \mid (\vec{x} - (\vec{\omega}_s + \varepsilon \vec{n})) \cdot \vec{n} = 0 \}, \quad (21)$$

where already an infinitesimal step in  $\varepsilon \vec{n}$  is taken. Furthermore, since we define the critical temperature to be the lower bound of the bisection interval, we have to ensure that the numerical minimization finds the symmetric global minimum. This is ensured by shifting the temperature by  $T_c + \delta T$  and so the temperature is above the critical temperature and the symmetric vacuum is the only global minimum of the potential. In this way we can ensure that the numerical minimization finds unambiguously the symmetric vacuum state  $\vec{\omega}_s$  with a unique phase. Note that  $\vec{\omega}_s$  corresponds to the found global minimum in the orthogonal plane defined in Eq. (21). The default values of the numerical parameters are chosen to be

$$\varepsilon = 10^{-2}, \quad \delta T = 1 \text{ GeV}. \quad (22)$$

It was explicitly checked that the impact of the chosen parameters has a negligible impact on the BAU prediction. Taking the straight line in the VEV vector space  $\{\vec{\omega}\}$  as a first guess allows us to go from one minimum to the other with a certain stepsize

$$\vec{\omega} \rightarrow \vec{\omega}^{(n)} \equiv \vec{\omega}(t_n), \quad (23)$$

where  $t_n$  determines the position after the  $n$ -th step. The orthogonal plane to the straight line in a given step point is defined by

$$\vec{\omega} \in \left\{ \vec{x} \mid \left( \vec{x} - \vec{\omega}^{(n)} \right) \cdot \vec{n} = 0 \right\}, \quad (24)$$

and allows to find the global minimum fulfilling Eq. (24). Successively, the global minima in the orthogonal planes are determined. These points create a grid that approximates the true tunnel path between the two degenerate minima. With the help of a cubic-spline path  $\gamma$  approximating the grid, the maximum of the effective one-loop potential at finite temperature along the approximated true tunnel path can be determined. The resulting barrier height is then given by

$$V_b = \max_{\vec{\omega} \in \gamma} (V_{\text{eff}}(\vec{\omega})) - V_{\text{eff}}(\vec{\omega}_b). \quad (25)$$

With the determination of the barrier height and the critical VEV  $v_c$  it is possible to parametrise the VEV configuration as a function of the bubble distance  $z$  by using Eq. (18). In CP-violating models the complex VEV configuration induces complex masses for fermions with Yukawa-like interactions where we parametrise the complex fermion masses as ( $i$  denotes the fermion species)

$$m_i(z) = |m_i(z)| \exp(i\theta(z)). \quad (26)$$

In BSMPT v2 the absolute value  $|m_i|$  and the phase factor  $\theta$  are determined numerically. The absolute value is determined by evaluating the mass matrix with the given VEV configuration at the wall distance  $z$ . The phase factor is determined by first evaluating the phase factor in the broken and symmetric minimum<sup>3</sup>, referred to as  $\theta_{\text{brk}}$  and  $\theta_{\text{sym}}$ , respectively, and then using the analogous of Eq. (18), yielding

$$\theta(z) = \left( \theta_{\text{brk}} - \frac{\theta_{\text{brk}} - \theta_{\text{sym}}}{2} \left( 1 + \tanh \frac{z}{L_W} \right) \right). \quad (27)$$

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<sup>3</sup>Note that we use  $\vec{\omega}_s$  for the symmetric vacuum configuration to ensure a unique phase of the symmetric vacuum.

### 3.2 Semi-Classical Force Approach

In the following section we give all necessary formulas for the numerical implementation of the semi-classical force approach, which we denote by FH. We do not comment on the actual derivation of the formulas and will refer to the corresponding literature [43–45]. For a phenomenological discussion of our implementation we refer to [51]. The BAU is calculated in a two-step approach, where in the first step the quantum transport equations are solved to obtain the left-handed fermion excess in front of the bubble wall. In the second step this left-handed fermion excess is translated to the actual baryon-asymmetry through an electroweak sphaleron transition.

The left-handed fermion excess (given in terms of the second-order CP-odd chemical potentials  $\mu_{x,2}$ ) triggering the electroweak sphaleron transition is given by

$$\mu_{BL} = \frac{1}{2} (1 + 4K_{1,t}) \mu_{t,2} + \frac{1}{2} (1 + 4K_{1,b}) \mu_{b,2} - 2K_{1,t} \mu_{t^c,2}, \quad (28)$$

where  $t(t^c)$  corresponds to the left-handed (charge conjugated right-handed) top quark and  $b$  to the bottom quark. The thermal transport coefficients, required here and in the following, are defined as

$$K_{1,i} = - \left\langle \frac{p_z^2}{E_0} \partial_E^2 f_{i,0} \right\rangle, \quad (29a)$$

$$K_{2,i} = \left\langle \frac{\partial_E^2 f_{i,0}}{2E_0} \right\rangle, \quad (29b)$$

$$K_{4,i} = \left\langle \frac{p_z^2}{E_0^2} \partial_E f_{i,0} \right\rangle, \quad (29c)$$

$$\tilde{K}_{5,i} = \left[ \frac{p_z^2}{E_0} \partial_E f_{i,0} \right], \quad (29d)$$

$$\tilde{K}_{6,i} = \left[ \frac{E_0^2 - p_z^2}{2E_0^3} \partial_E f_{i,0} \right], \quad (29e)$$

$$K_{8,i} = \left\langle \frac{|p_z| \partial_E f_{i,0}}{2E_0^2 E_{0z}} \right\rangle, \quad (29f)$$

$$K_{9,i} = \left\langle \frac{|p_z|}{4E_0^3 E_{0z}} \left( \frac{\partial_E f_{i,0}}{E_0} - \partial_E^2 f_{i,0} \right) \right\rangle, \quad (29g)$$

where

$$E_0(z) = \sqrt{p_x^2 + p_y^2 + p_z^2 + m(z)^2}, \quad (30)$$

$$E_{0z} = \sqrt{p_z^2 + m(z)^2}, \quad (31)$$

are the energies of the quasi-particles in front of the bubble wall. Here  $\partial_E$  denotes the partial derivative with respect to the energy of the distribution function. The expectation values are given by

$$\langle X \rangle = \frac{\int d^3p X(p)}{\int d^3p \partial_E f_{0+}(m=0)}, \quad [X] = \frac{\int d^3p X(p)}{\int d^3p f_{i,0,vW}} = \frac{\int d^3p X(p)}{\int d^3p f_{i,0}}, \quad (32)$$

and the distribution functions are given by

$$f_{i,0} = f_i|_{\mu_i=0, \delta f_i=0, v_W=0}, \quad f_{0+} = f_i|_{i=\text{fermion}, \mu_i=0, \delta f_i=0, v_W=0}, \quad f_{i,0,v_W} = f_{i,0} + v_W p_z \partial_{E_0} f_{i,0}. \quad (33)$$

Note that we do not use the complete dependence on the wall velocity  $v_W$  in the thermal coefficients induced by the distribution function (+ refers to fermions, - to bosons,  $\beta = 1/T$ )

$$f_i = \frac{1}{\exp(\beta[\gamma_W(E_0 + v_W p_z) - \mu_i]) \pm 1} + \delta f_i \quad (34)$$

with

$$\gamma_W = \frac{1}{\sqrt{1 - v_W^2}}, \quad (35)$$

and the small perturbation  $\delta f_i$ . Instead, the additional assumption of small wall velocities ( $v_W \ll 1$ ) is used to expand the thermal coefficients, simplifying the transport equations further. In this way, it is not possible to discuss the behaviour for arbitrary wall velocities, and wall velocities with values close to the plasma speed should be taken with caution. Recently, Ref. [50] extended the semi-classical force approach for arbitrary wall velocities. Furthermore, Ref. [80] also improved the fluid approach to relativistic wall velocities.

The thermal coefficients are evaluated in an equidistant grid in  $\{m^2(z), T\}$  which is called through a bi-cubic spline in BSMPT v2. Thereby it is possible to keep the  $z$  dependence in the thermal coefficients without significant increase of run-time. More specifically, we sampled  $m^2$  from 0 GeV<sup>2</sup> to 5 GeV<sup>2</sup> with a step size of  $10^{-3}$  and afterwards up to 200<sup>2</sup> GeV<sup>2</sup> with a step size of 5 GeV<sup>2</sup>. The temperature steps are sampled from 10 GeV up 250 GeV with a step size of 2 GeV. We tested several different step sizes in the grid and observed that the overall result of the BAU does not show a significant dependence. The effect was in the sub-percentage region at most. The choice was a compromise between the header file size due to the larger grid and the required precision.<sup>4</sup>

In the thermal plasma in front of the bubble wall, the full particle content has to be considered in the transport equations. The dominant contribution to the production of the baryon asymmetry is given by the top quark, however, because of its large mass, or rather its strong Yukawa interaction with the thermal plasma. It is the (large) amount of CP violation in the quark sector that dominantly drives the generation of the left-handed excess.

The transport equations are derived for a single Dirac fermion with a complex mass term and include Yukawa interactions, strong sphaleron interactions and  $W$ -boson scattering. The

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<sup>4</sup>Information on the grid can also be found at the webpage in [https://phbasler.github.io/BSMPT/Kfunctions\\_grid.8h.html](https://phbasler.github.io/BSMPT/Kfunctions_grid.8h.html).

transport equations read [43, 44]

$$\begin{aligned}
0 = & 3v_W K_{1,t} (\partial_z \mu_{t,2}) + 3v_W K_{2,t} (\partial_z m_t^2) \mu_{t,2} + 3 (\partial_z u_{t,2}) \\
& - 3\Gamma_y (\mu_{t,2} + \mu_{t^c,2} + \mu_{h,2}) - 6\Gamma_M (\mu_{t,2} + \mu_{t^c,2}) - 3\Gamma_W (\mu_{t,2} - \mu_{b,2}) \\
& - 3\Gamma_{ss} [(1 + 9K_{1,t}) \mu_{t,2} + (1 + 9K_{1,b}) \mu_{b,2} + (1 - 9K_{1,t}) \mu_{t^c,2}] , 
\end{aligned} \tag{36a}$$

$$\begin{aligned}
0 = & 3v_W K_{1,b} (\partial_z \mu_{b,2}) + 3 (\partial_z u_{b,2}) - 3\Gamma_y (\mu_{b,2} + \mu_{t^c,2} + \mu_{h,2}) - 3\Gamma_W (\mu_{b,2} - \mu_{t,2}) \\
& - 3\Gamma_{ss} [(1 + 9K_{1,t}) \mu_{t,2} + (1 + 9K_{1,b}) \mu_{b,2} + (1 - 9K_{1,t}) \mu_{t^c,2}] , 
\end{aligned} \tag{36b}$$

$$\begin{aligned}
0 = & 3v_W K_{1,t} (\partial_z \mu_{t^c,2}) + 3v_W K_{2,t} (\partial_z m_t^2) \mu_{t^c,2} + 3 (\partial_z u_{t^c,2}) \\
& - 3\Gamma_y (\mu_{t,2} + \mu_{b,2} + 2\mu_{t^c,2} + 2\mu_{h,2}) - 6\Gamma_M (\mu_{t,2} + \mu_{t^c,2}) \\
& - 3\Gamma_{ss} [(1 + 9K_{1,t}) \mu_{t,2} + (1 + 9K_{1,b}) \mu_{b,2} + (1 - 9K_{1,t}) \mu_{t^c,2}] , 
\end{aligned} \tag{36c}$$

$$0 = 4v_W K_{1,h} (\partial_z \mu_{h,2}) + 4 (\partial_z u_{h,2}) - 3\Gamma_y (\mu_{t,2} + \mu_{b,2} + 2\mu_{t^c,2} + 2\mu_{h,2}) - 4\Gamma_h \mu_{h,2} , \tag{36d}$$

$$S_t = -3K_{4,t} (\partial_z \mu_{t,2}) + 3v_W \tilde{K}_{5,t} (\partial_z u_{t,2}) + 3v_W \tilde{K}_{6,t} (\partial_z m_t^2) u_{t,2} + 3\Gamma_t^{\text{tot}} u_{t,2} , \tag{36e}$$

$$0 = -3K_{4,b} (\partial_z \mu_{b,2}) + 3v_W \tilde{K}_{5,b} (\partial_z u_{b,2}) + 3\Gamma_b^{\text{tot}} u_{b,2} , \tag{36f}$$

$$S_t = -3K_{4,t} (\partial_z \mu_{t^c,2}) + 3v_W \tilde{K}_{5,t} (\partial_z u_{t^c,2}) + 3v_W \tilde{K}_{6,t} (\partial_z m_t^2) u_{t^c,2} + 3\Gamma_t^{\text{tot}} u_{t^c,2} , \tag{36g}$$

$$0 = -4K_{4,h} (\partial_z \mu_{h,2}) + 4v_W \tilde{K}_{5,h} (\partial_z u_{h,2}) + 4\Gamma_h^{\text{tot}} u_{h,2} . \tag{36h}$$

The second-order CP-odd chemical potentials  $\mu_{i,2}$  ( $i = t, b, t^c, h$ ) describe the particle density excess of the left-handed top and bottom quarks, the right-handed top quark and the Higgs boson. The plasma velocities  $u_i$  are defined as in Ref. [43]. The source term  $S_t$  reads

$$S_t = -v_W K_{8,t} \partial_z (m_t^2 \partial_z \theta) + v_W K_{9,t} (\partial_z \theta) m_t^2 (\partial_z m_t^2) . \tag{37}$$

The Yukawa interaction rate for the top quark,  $\Gamma_y$ , and the strong sphaleron rate  $\Gamma_{ss}$  are given by [43]

$$\Gamma_y = 4.2 \cdot 10^{-3} T_c , \quad \Gamma_{ss} = 4.9 \cdot 10^{-4} T_c , \tag{38}$$

and the Higgs number violating rate is given by

$$\Gamma_h = \frac{m_W^2(z, T_c)}{50T_c} . \tag{39}$$

The  $W$ -boson mass  $m_W$  is determined at given  $z$  and for the critical temperature  $T_c$  from the numerical evaluation of the gauge boson mass matrix. The top-helicity flipping rate is implemented as

$$\Gamma_M = \frac{m_t^2(z, T_c)}{63T_c} . \tag{40}$$

The total quark and Higgs interaction rates can be determined with the help of their respective diffusion constants,

$$\Gamma_t^{\text{tot}} = \frac{K_{4,t}}{K_{1,t} D_t} , \quad \Gamma_b^{\text{tot}} = \frac{K_{4,b}}{K_{1,b} D_b} , \quad \Gamma_h^{\text{tot}} = \frac{K_{4,h}}{K_{1,h} D_h} , \tag{41}$$

with the diffusion constants for the top and bottom quarks ( $q = t, b$ ) and the Higgs boson given by [62, 63]

$$D_q = \frac{6}{T_c} \quad \text{and} \quad D_h = \frac{20}{T_c} . \tag{42}$$

The  $W$ -scattering rate is approximated by the total Higgs interaction rate  $\Gamma_W = \Gamma_h^{\text{tot}}$ . It should be emphasized that all interaction rates are calculated in the plasma frame. The transport equations in Eq. (36) are implemented in `BSMPT v2` and solved with the help of the `C++` numerical library `boost` [64], where all chemical potentials and the plasma velocities are assumed to vanish at infinite distance to the bubble wall in the symmetric phase (positive  $z$ ), for which the default numerical value is set equal to four times the bubble wall thickness  $L_W$ . The user can choose, however, any other value. It was checked numerically that the choice of  $z_{\text{max}} = 4L_W$  [65] for the boundary condition is on the one hand numerically stable and on the other hand does not significantly change the result.

As a second alternative variant of the transport equations, the plasma velocities in Eq. (36) are expressed through the derivatives of Eqs. (36e) to (36h). In doing so, the derivatives of the thermal coefficients are dropped, moreover derivatives of third or higher order are neglected, allowing to express the plasma velocities as

$$\partial_z u_{t,2} = \frac{\partial_z S_t + 3K_{4,t} \partial_z^2 \mu_{t,2}}{3(\Gamma_t^{\text{tot}} + K_{6,t} v_W \partial_z m_t^2)}, \quad (43a)$$

$$\partial_z u_{t^c,2} = \frac{\partial_z S_t + 3K_{4,t} \partial_z^2 \mu_{t^c,2}}{3(\Gamma_t^{\text{tot}} + K_{6,t} v_W \partial_z m_t^2)}, \quad (43b)$$

$$\partial_z u_{b,2} = \frac{K_{4,b}}{\Gamma_b^{\text{tot}}} \partial_z^2 \mu_{b,2}, \quad (43c)$$

$$\partial_z u_{h,2} = \frac{K_{4,h}}{\Gamma_h^{\text{tot}}} \partial_z^2 \mu_{h,2}, \quad (43d)$$

and the source term as

$$\partial_z S_t = v_W K_{9,t} (m_t^2 \partial_z^2 \theta + \partial_z \theta \partial_z m_t^2) \partial_z m_t^2 - 2v_W K_{8,t} \partial_z m_t^2 \partial_z^2 \theta. \quad (44)$$

These expressions for the plasma velocities allow to formulate the transport equations as a differential system of equations of second order. As boundary conditions analogous conditions as in the previous approach are chosen. The chemical potentials and their derivatives are assumed to vanish at  $z_{\text{max}} = 4L_W$ .

Equation (28) allows to determine the produced BAU by evaluating the integral

$$\eta_B = \frac{405\Gamma_{ws}}{4\pi^2 v_W g_* T} \int_0^\infty dz \mu_{BL}(z) \exp\left(-\frac{45\Gamma_{ws}}{4v_W} z\right) \quad (45)$$

numerically, where  $g_* = 106.75$  is the effective number of degrees of freedom in the plasma [63,66],  $v_W$  the wall velocity and  $\Gamma_{ws}$  is the weak sphaleron rate, given by [67–69]

$$\Gamma_{ws} = 10^{-6} T. \quad (46)$$

### 3.3 VEV-insertion Method/Fluid Equation

As a second approach for the calculation of the BAU the VEV-insertion method (VIA) is chosen. The VIA can be understood as an expansion in  $v(z)/T$  in which the fermionic two-point function is expanded. This approach allows also to include further lighter quarks and leptons in the transport equations. Leptons do not suffer from the strong sphaleron suppression and their

diffusion constant is significantly larger compared to that of the quarks, allowing for a more efficient diffusion process. Furthermore, in some specific models and parameter regions the lepton interaction rates are enhanced so that a sufficiently large BAU can be produced through leptons [70]. In `BSMPT v2` the inclusion of the dominant lepton contribution from the  $\tau$  leptons and of the contributions from the two heaviest quarks,  $t$  and  $b$ , is possible.

The implementation of the transport equations follows Ref. [49, 78] and is adapted accordingly. The chemical potentials for the particles contributing to the system of transport equations are expressed as net chemical potentials, meaning that in the following  $\mu^{(x)}$  refers to the chemical potential of the particles  $x$  minus the one of their anti-particles. We denote the net number densities<sup>5</sup> of the left- and right-handed quark/lepton and scalar degrees of freedom by

$$\begin{aligned} n_q &= n_{t_L} + n_{b_L}, & n_t &= n_{t_R}, & n_b &= n_{b_R}, \\ n_l &= n_{\nu_L} + n_{\tau_L}, & n_\tau &= n_{\tau_R}, & n_\nu &= n_{\nu_R}, \\ n_{h_k} &= n_{h_k^0} + n_{h_k^\pm}. \end{aligned} \quad (47)$$

The index  $k$  counts the doublets  $\Phi_k = (h_k^\pm, h_k^0)$  considered in the model under investigation. The strong sphaleron interactions allow to relate the light quark densities via

$$n_{q_1} = n_{q_2} = -2n_u = -2n_d = -2n_s = -2n_c \quad (48)$$

so that only one of them needs to be considered, which we choose to be  $n_u$ . The transport equations including the dominant quark contributions of  $t, b$ , the contribution of the  $\tau$  lepton as well as the neutrino, the light quarks and the Higgs contributions are given by [49]

$$\partial_\mu j_q^\mu = +\Gamma_M^{(t)} \mu_M^{(t)} + \Gamma_M^{(b)} \mu_M^{(b)} + \Gamma_Y^{(t)} \mu_Y^{(t)} + \Gamma_Y^{(b)} \mu_Y^{(b)} - 2\Gamma_{ss} \mu_{ss} - S_{\mathcal{CP}}^{(t)} - S_{\mathcal{CP}}^{(b)} \quad (49a)$$

$$\partial_\mu j_t^\mu = -\Gamma_M^{(t)} \mu_M^{(t)} - \Gamma_Y^{(t)} \mu_Y^{(t)} + \Gamma_{ss} \mu_{ss} + S_{\mathcal{CP}}^{(t)} \quad (49b)$$

$$\partial_\mu j_b^\mu = -\Gamma_M^{(b)} \mu_M^{(b)} - \Gamma_Y^{(b)} \mu_Y^{(b)} + \Gamma_{ss} \mu_{ss} + S_{\mathcal{CP}}^{(b)} \quad (49c)$$

$$\partial_\mu j_l^\mu = +\Gamma_M^{(\tau)} \mu_M^{(\tau)} + \Gamma_Y^{(\tau)} \mu_Y^{(\tau)} - S_{\mathcal{CP}}^{(\tau)} \quad (49d)$$

$$\partial_\mu j_\nu^\mu = 0 \quad (49e)$$

$$\partial_\mu j_\tau^\mu = -\Gamma_M^{(\tau)} \mu_M^{(\tau)} - \Gamma_Y^{(\tau)} \mu_Y^{(\tau)} + S_{\mathcal{CP}}^{(\tau)} \quad (49f)$$

$$\partial_\mu j_{h_k}^\mu = +\Gamma_Y^{(t)} \mu_Y^{(t)} - \Gamma_Y^{(b)} \mu_Y^{(b)} + \Gamma_Y^{(u)} \mu_Y^{(u)} - \Gamma_Y^{(\tau)} \mu_Y^{(\tau)} \quad (49g)$$

$$\partial_\mu j_u^\mu = +\Gamma_{ss} \mu_{ss}. \quad (49h)$$

As noted above, here the distribution function of the up quark is chosen.

The left-hand side of Eq. (49) can be expressed in the rest frame of the wall as

$$\partial_\mu j_i^\mu(x) \approx v_W n_i' - D_i \nabla^2 n_i \approx v_W n_i' - D_i n_i'' \quad (i = q, t, b, l, \nu, \tau, h_k, u), \quad (50)$$

with the diffusion constants for the quarks given by

$$D_q = \frac{6}{T_C}. \quad (51)$$

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<sup>5</sup>Note that the chemical potentials  $\mu$  and the particle densities  $n$  are related through the high-temperature expansion,  $n = \frac{T^2}{6} \kappa \mu + \mathcal{O}(\mu^3)$ , with the statistical factor  $\kappa$  defined below.

The diffusion constants for the left-handed leptons are implemented as

$$D_l = \frac{100}{T_c} \quad (52)$$

and the diffusion constant for the right-handed  $\tau$  as

$$D_\tau = \frac{380}{T_c} . \quad (53)$$

The single and double derivatives denoted by prime(s) are taken with respect to the bubble wall distance  $z$ . The diffusion constant for the Higgs bosons is taken as

$$D_{h_k} = \frac{100}{T_c} . \quad (54)$$

The strong sphaleron rate is given by

$$\Gamma_{ss} = 14\alpha_s^4 T_c , \quad (55)$$

and the Yukawa rates of the quarks are implemented as [71]

$$\Gamma_Y^{(q)} = 0.19\alpha_s y_q^2 T_c , \quad (56)$$

where  $\alpha_s$  denotes the strong coupling constant and  $y_q$  the zero-temperature Yukawa strength. The Yukawa interaction rate for the  $\tau$  lepton is given by

$$\Gamma_Y^{(\tau)} = 0.28\alpha_w y_\tau^2 T_c , \quad (57)$$

with  $\alpha_w = g_2^2/(4\pi)$ , where  $g_2$  denotes the SU(2) gauge coupling, and the zero-temperature Yukawa strength  $y_\tau$ .

The chemical potentials on the right-hand side of Eq. (49) are combinations of the net chemical potentials of the particles and are given by

$$\mu_M^{(t)} = \left( \frac{n_t}{\kappa_t} - \frac{n_q}{\kappa_q} \right) , \quad \mu_Y^{(t)} = \left( \frac{n_t}{\kappa_t} - \frac{n_q}{\kappa_q} - \sum_k \frac{n_{h_k}}{\kappa_{h_k}} \right) , \quad (58)$$

$$\mu_M^{(b)} = \left( \frac{n_b}{\kappa_b} - \frac{n_q}{\kappa_q} \right) , \quad \mu_Y^{(b)} = \left( \frac{n_b}{\kappa_b} - \frac{n_q}{\kappa_q} + \sum_k \frac{n_{h_k}}{\kappa_{h_k}} \right) , \quad (59)$$

$$\mu_M^{(\tau)} = \left( \frac{n_\tau}{\kappa_\tau} - \frac{n_l}{\kappa_l} \right) , \quad \mu_Y^{(\tau)} = \left( \frac{n_\tau}{\kappa_\tau} - \frac{n_l}{\kappa_l} + \sum_k \frac{n_{h_k}}{\kappa_{h_k}} \right) , \quad (60)$$

$$\mu_{ss} = \left( \frac{2n_q}{\kappa_q} - \frac{n_t}{\kappa_t} - \frac{n_b}{\kappa_b} - \frac{8n_u}{\kappa_L} - \frac{4n_u}{\kappa_R} \right) , \quad (61)$$

where the chemical potentials are rescaled with a factor of  $6/T^2$ . This factor is absorbed in the interactions rates. The statistical factor  $\kappa_L$  ( $\kappa_R$ ) corresponds to the statistical factor of a massless left (right)-handed quark. The right-handed CP-violating source term is implemented

as ( $i = t, b, \tau$ )

$$S_{\mathcal{CP}}^{(i)} = \frac{N_c v_W}{\pi^2} \text{Im}(f_i' f_i^*) \int dk \frac{k^4}{\omega^4} \left[ -\frac{\Gamma_T}{2\omega} + \frac{5\Gamma_T}{4\omega^2} \delta\omega + \left( \frac{\Gamma_T}{\omega} - \frac{5\Gamma_T \delta\omega}{2\omega^2} \right) n(\omega) \right. \\ \left. + \left( \frac{-\omega^2}{2\Gamma_T} + \frac{\omega^4}{2k^2 \Gamma_T} - \frac{\Gamma_T}{2} + \left( \frac{\omega}{2\Gamma_T} + \frac{3\Gamma_T}{2\omega} \right) \delta\omega \right) n'(\omega) \right] \\ + \mathcal{O} \left( \delta\omega^2; \left( \frac{\Gamma_T}{T} \right)^2; n'' \right), \quad (62)$$

with the colour factor  $N_c = 3(1)$  for top, bottom ( $\tau$ ), and  $k$  denoting the four-momentum of particle  $i$ . Note that, for better readability, we neglect the index  $i$  in  $n$ ,  $k$  and  $\omega$  (which is defined below). The Yukawa interaction strength  $f_i$  corresponds to the interaction of the left- and right-handed fermions in the Lagrangian

$$\mathcal{L} \supset -\frac{f_i(T, \phi_b)}{\sqrt{2}} \bar{\Psi}_L^i \Psi_R^i + \text{h.c.}, \quad (63)$$

depending on the background Higgs field configuration  $\phi_b$  and thermal interactions.  $f_i(T, \phi_b)$  can be split in one part containing the contribution from the one-loop corrected mass at zero temperature and another part containing the thermal mass contributions. We use the following thermal masses for quarks ( $q$ ) and leptons ( $l$ ), respectively, [72]

$$\left( m_{T,R}^q \right)^2 = \left( \frac{g_1^2}{18} + \frac{g_3^2}{6} + \frac{y_q^2}{8} \right) T^2, \quad (64a)$$

$$(\delta m^q)^2 \equiv \left( m_{T,R}^q \right)^2 - \left( m_{T,L}^q \right)^2 = \left( \frac{5g_1^2}{96} - \frac{3g_2^2}{32} + \frac{y_q^2}{16} \right) T^2, \quad (64b)$$

$$\left( m_{T,R}^l \right)^2 = \left( \frac{g_1^2}{8} + \frac{y_l^2}{8} \right) T^2, \quad (64c)$$

$$(\delta m^l)^2 \equiv \left( m_{T,R}^l \right)^2 - \left( m_{T,L}^l \right)^2 = \left( \frac{3g_1^2}{32} - \frac{3g_2^2}{32} + \frac{y_l^2}{16} \right) T^2, \quad (64d)$$

with the SM gauge couplings  $g_1, g_2, g_3$  and the zero-temperature Yukawa couplings  $y_q, y_l$ . The gauge coupling  $g_1$  is not GUT normalised. We chose to parametrise the source terms and relaxation rates  $\Gamma_M^{(i)}$  in terms of the respective right-handed mass and the mass difference  $\delta m$  to the corresponding left-handed mass. This allows us to expand the source terms and relaxation rates in  $\delta m$ . The dispersion of the left( $L$ )-/right( $R$ )-handed particle  $i$  entering the source term is given by

$$\epsilon_{L/R}^i = \omega_{L/R}^i + i\Gamma_{T,L/R}^i \equiv \sqrt{(k^i)^2 + \left( m_{T,L/R}^i \right)^2} - i\Gamma_{T,L/R}^i. \quad (65)$$

The thermal width is approximately the same for all particles  $i = t, b, \tau$  and given by (the index  $i$  can be dropped)

$$\Gamma_{T,L} \approx \Gamma_{T,R} \approx \Gamma_T \approx 0.16T. \quad (66)$$

Furthermore, the source term in Eq. (62) was expanded for small  $\Gamma_T/T \ll 1$ . The Fermi-Dirac distribution function is given by

$$n(x) = (e^x + 1)^{-1}, \quad (67)$$

and the expansion parameter  $\delta\omega^i$  by

$$\delta\omega^i = \frac{(\delta m^i)^2}{2\sqrt{(k^i)^2 + (m_R^i)^2}}. \quad (68)$$

Analogously, the relaxation rates are expanded for small thermal widths  $\Gamma_T$  and small differences in the left- and right-handed thermal masses and implemented as

$$\Gamma_M^{(i)} = \frac{6}{T^2} \cdot \frac{N_c}{2\pi^2 T} |f_i|^2 \int \frac{dk k^2}{\omega^2} \left( -\frac{k^2}{\Gamma_T} + \frac{\omega^2}{\Gamma_T} + \frac{k^2 \Gamma_T}{\omega^2} + \left( \frac{k^2}{\omega \Gamma_T} - \frac{2k^2 \Gamma_T}{\omega^3} \right) \delta\omega \right) h(\omega) \quad (69)$$

$$+ \mathcal{O} \left( \delta\omega^2; \left( \frac{\Gamma_T}{T} \right)^2; h' \right),$$

with

$$h(x) = e^x / (e^x + 1)^2, \quad (70)$$

and where again we suppressed the index  $i$  in  $k$ ,  $\omega$  and  $\delta\omega$  for better readability. The scale factor of  $\frac{6}{T^2}$  from the high-temperature expansion of the chemical potentials is absorbed in the relaxation rates. The high-temperature expansion of the chemical potential  $\mu$  yields the following relation between the chemical potential  $\mu$  of the particle and its number density  $n$ ,

$$n = \frac{T^2}{6} \mu \kappa + \mathcal{O}(\mu^3), \quad (71)$$

with the statistical factor for fermions ( $F, +$ ) and bosons ( $B, -$ ), respectively,

$$\kappa(x) = \kappa(0) \frac{c_{F,B}}{\pi^2} \int_{m/T}^{\infty} dx \frac{x e^x}{(e^x \pm 1)^2} \sqrt{x^2 - m^2/T^2}, \quad (72)$$

where the numerical values for the normalisation are given by  $c_F = 6$  and  $c_B = 3$ .

All integrals over the momentum  $k$  above are evaluated numerically in `BSMPT v2` in the range of  $k \in [0, 10^4]$ . The upper boundary is chosen such that a numerically stable result can be obtained and at the same time the result does not depend significantly on the chosen cut. The differential system of equations in Eq. (49) is solved with the help of the `boost` library at a given distance  $z$ . Analogously to the `FH` approach the boundary condition is chosen such that the chemical potentials vanish at  $z_{max} = 4L_W$ . The resulting grid of the sum of all left-handed quarks and leptons [49],

$$n_L^0(z) \approx (n_q - 4n_u + n_l), \quad (73)$$

is interpolated as cubic spline and finally, the following differential equation is integrated to determine the produced baryon density  $n_B$

$$v_W n_B' - D_q n_B'' = -\Gamma_{ws} \left( \frac{3}{2} n_L^0 + \mathcal{R} n_B \right). \quad (74)$$

The electroweak sphaleron transition rate is implemented as

$$\Gamma_{ws} = 6\kappa \alpha_w^5 T_c \approx 5 \cdot 10^{-6} T_c, \quad (75)$$

with the numerical factors  $\kappa \approx 20$  and  $\mathcal{R} = \frac{15}{4}$ .

## 4 Program Description

In this section, we describe the system requirements for BSMPT v2 and provide a guide for installing and using the program.

### 4.1 System Requirements

The program was developed and tested on OpenSuse 42.2, Ubuntu 14.04, Ubuntu 16.04, Ubuntu 19.10, Ubuntu 20.04 and Mac 10.13 with g++ v6.2.1, g++ v.7.2.1, g++ v.9.3.0 and g++ 10.2.0. The program can be downloaded at:

<https://github.com/phbasler/BSMPT>

For a working version of BSMPT v2 the following dependencies are required:

- CMake v3.13 or higher. It can be installed either through pip or directly from <https://cmake.org/download/>.
- The GNU Scientific Library (GSL) [73] v2.1 or higher is assumed to be installed in PATH. GSL is required for the calculation of the Riemann- $\zeta$  functions, the double factorial and for the minimization.
- Eigen3 v3.3 [74] or higher is used to calculate the eigenvalues and eigenvectors of the mass matrices.
- Boost 1.66 [64] is required for the computation of the BAU. For the calculation of the phase transition the Boost library is optional.

Furthermore, at least one of the following two libraries has to be provided

- libcmaes [75]. Per default BSMPT will install libcmaes in the build directory, which is recommended for proper links to Eigen3.
- NLOpt [76] using the DIRECT-L [77] algorithm. As an additional option for the minimization we provide a link to NLOpt.

### 4.2 Download

The latest stable version of the program package BSMPT v2 can be obtained from

<https://github.com/phbasler/BSMPT> .

We also provide a Doxygen documentation there which incorporates all functions and parameters of BSMPT v2. The user can either clone the repository or download the package as a zip archive. The chosen directory of the user is referred to as \$BSMPT in the following. The main directory contains the following subdirectories:

- example** In this subfolder sample input files needed for the binaries are provided.
- manual** This subfolder contains a copy of the manual of BSMPT kept up to date with changes in the code. Additionally, we include the **changelog** file documenting corrected bugs and modifications of the program.
- sh** In this subdirectory the python files **prepareData\_XXX.py** (XXX= R2HDM,

C2HDM, N2HDM) are provided allowing to order the data sample according to the input requirements.

<code>src</code>	This subfolder contains the source files of the code.
<code>include</code>	This subfolder contains the header files of the code.
<code>tools</code>	This folder contains configurations for the installation with <code>cmake</code> .
<code>maple</code>	This folder contains a Maple worksheet template which can be used to calculate the necessary tensors to implement a new model in BSMPT.

The subfolders of `src` contain the following files:

<code>src/minimizer</code>	This directory contains the minimization routines.
<code>src/models</code>	This directory contains all implemented models. If a new model is added it must be added in this folder. A template class with instructions on how to add a new model and the file <code>SMparam.h</code> with the Standard Model parameters are provided.
<code>src/prog</code>	This directory contains the source code for the executables.
<code>src/ThermalFunctions</code>	This directory contains the implementation of the thermal integrals.
<code>src/WallThickness</code>	This directory contains the calculation of the wall thickness.
<code>src/Kfactors</code>	This directory contains the calculation and interpolation of the thermal transport coefficients $K_i$ used in one of the implemented calculations of the BAU.
<code>src/baryo_calculations</code>	This directory contains the implementation of the different approaches to calculate the BAU.

### 4.3 Installation

The compilation requires a C++ compiler supporting the C++14 standard. To install BSMPT v2 the following steps have to be performed:

1. In the directory `$BSMPT` call

```
1 mkdir build && cd build
```

2. In order to generate the makefile call

```
2 cmake [OPTIONS] ..
```

in `$BSMTP/build` with the following possible options

- `CXX=C++Compiler` If not given the default compiler will be used.
- `-DEigen3_DIR=/path/to/eigen3Installation/share/eigen3/cmake` Sets the path to the Eigen3 installation. Can be used in case Eigen3 is not found automatically.
- `-Dlibcmaes_ROOT=/path/to/libcmaesInstallation` if libcmaes is installed previously.
- `-DUseLibCMAES=ON/OFF`, where the default is ON. Switch to decide if libcmaes should be used or not.

- `-DNlopt_Dir=/path/to/NloptInstallation` This gives the corresponding path to the Nlopt installation if Nlopt is not found automatically.
- `-DUseNlopt=ON/OFF`, default is ON. Switch to decide if Nlopt should be used or not.
- `-DBoost_ROOT=/path/to/boost` This is only necessary if Boost is not found automatically through cmake.

A complete call would look like:

```
3 CXX=C++Compiler cmake -DEigen3_DIR=/path/to/eigen3Installation/share/
  eigen3/cmake -Dlibcmaes_ROOT=/path/to/libcmaesInstallation -DNlopt_Dir
  =/path/to/NloptInstallation -DBoost_ROOT=/path/to/boost ..
```

### 3. Subsequently call

```
1 cmake --build .
```

If the installation is successful, the executables `BSMPT`, `CalcCT`, `NLOVEV`, `VEVEVO`, `Test`, `TripleHiggsCouplingsNLO`, `CalculateEWBG`, `PlotEWBG_vw`, and `PlotEWBG_nL` are generated in `$BSMPT/build/bin/`.

- (Optional) Furthermore, we provide a detailed documentation of each function implemented in `BSMPT v2` through doxygen. To generate the doxygen documentation call in `$BSMPT/build`

```
1 cmake --build . -t doc
```

Afterwards, the documentation can be found as `$BSMPT/build/html/index.html`. Note that for the generation of the documentation the program package doxygen is required.

- (Optional) We provide a unit-test, allowing the users to test their current installation of `BSMPT v2`. To perform the unit-test call in `$BSMPT/build/`

```
1 ctest
```

The test calls subsequently test frames checking for various quantities *e.g.* the NLO VEV configuration of a known benchmark scenario. So far, there are test frames available for the C2HDM, N2HDM and R2HDM. A relative agreement of the order  $\mathcal{O}(10^{-4})$  is demanded in each tested quantity. Note that the effective potential is not sensitive to the sign of the VEV configuration due to the  $SU(2)$  symmetry, hence the output of the minimization routines might differ in the sign of the VEVs. The absolute values, however, must be in agreement with the default values provided for the test frames.

## 4.4 Program Usage

In the following the different executables of `BSMPT v2` are described. All executables of `BSMPT v2` need the following additional input parameters

- *Model*: Input parameter to choose the model. Implemented are the CP-violating 2HDM ("`c2hdm`"), CP-conserving 2HDM ("`r2hdm`") and the CP-conserving N2HDM ("`n2hdm`"). With the release of `BSMPT v2` also the complex singlet extension ("`cxsm`") is added.

- *Inputfile*: sets the path and the name of the input file. The program expects the first line in the input file to be a header with the column names. Every following line then corresponds to the input of one particular parameter point. The parameters are required to be those of the Lagrangian in the interaction basis. If a different format for the input parameters is desired one needs to adapt the function `ReadAndSet` in the corresponding model file in `$BSMPT/src/models`. Note, that the program expects the input parameters to be separated by a tabulator. In the folder `$BSMPT/sh/`, we provide `python` scripts that prepare the data accordingly.
- *Outputfile*: sets the path and the name of the generated output file. We note, that the program does not create new folders so the user has to ensure the existence of the output directory.

Furthermore, every executable has a help menu which can be called by

```
4 ./executable --help
```

In addition to the given parameters here, the help menu will show an additional method for calling the executables with more options, e.g. turning off the minimizers at runtime. It is possible to switch the treatment of the thermal corrections from the default choice, referred to as Arnold Espinosa method, to the alternative method, referred to as Parwani method, by changing the variable `C_UseParwani` to true in the file

`$BSMPT/include/BSMPT/models/ClassPotentialOrigin.h`.

The changes have to be applied to the binaries through recompiling the code with `make` in the directory `$BSMPT/build`. In the following subsections we list the binaries of BSMPT v2.

#### 4.4.1 Test

`Test` provides a test binary to automatically check for implementation errors *e.g.* for new model implementations or changes in the source code. The following checks are performed by the binary:

- It checks if the tree-level minimum is given by the input value of  $v \approx 246.22$  GeV within the numerical precision.
- It compares between the masses of the quarks and gauge bosons given in the `SMparam.h` file and the internally calculated numerical values.
- It minimizes the tree-level potential and checks if the input minimum is the global minimum.
- It checks if the implemented simplified tree-level and counterterm potentials yield the same results as the generic potential.
- It checks if the number of labels in `addLegendCT`, `addLegendVEV`, `addLegendTemp` matches with the required number of counterterm parameters and VEVs.
- It checks if the higher-order Higgs boson masses obtained with the implemented counterterm potential are the same as the tree-level ones.

The test binary can be executed with

### Test

```
./bin/Test Model Inputfile Line
```

*Model* specifies the model under investigation. The line number of the parameter point which should be used for the test is given by *Line*. The results and status of the test will be prompted as terminal output. An example call for the C2HDM would look like

```
1 ./bin/Test c2hdm ../example/C2HDM_Input.dat output.csv 2
```

where the second line of `C2HDM_Input.dat` would be used.

In the following, we will list the executables and their individual function. Some of these executables are already present in the previous version of BSMPT. For completeness, we list them here as well. The new executables in BSMPT are `CalculateEWBG`, `PlotEWBG_vw`, and `PlotEWBG_nL` described in Secs. 4.4.7 to 4.4.9 in the following.

#### 4.4.2 BSMPT

BSMPT is the executable calculating the strength of the electroweak phase transition of a given parameter point in *Inputfile*. The binary is called by

### BSMPT

```
./bin/BSMPT Model Inputfile Outputfile LineStart LineEnd
```

Here and wherever they appear in the command lines in the following, *LineStart* and *LineEnd* set the line numbers of the first and the last parameter point provided in *Inputfile* for which the various quantities are to be calculated by BSMPT v2. Note that the first line of the input file is expected to be the header, so that the first parameter point should have the *LineStart* = 2. To calculate a single parameter point *LineStart* and *LineEnd* have to be equal. The results of BSMPT are written in *Outputfile* where the parameter point read in is extended by the results of the calculation. Also the legend from the input file is extended by the additional legend needed for the output. Every parameter point in the range of *LineStart* to *LineEnd* will be calculated and written to *Outputfile* regardless if the parameter point provides an SFOEWPT or not. An example call for the C2HDM would look like

```
1 ./bin/BSMPT c2hdm ../example/C2HDM_Input.dat output.csv 2 2
```

where the first data line of `C2HDM_Input.dat` would be used. The output file `output.csv` should be the same as `example/C2HDM_Input.dat_BSMPT` up to numerical fluctuations.

The column `omega_c/T_c` provides the information if the respective parameter points fulfill all checked conditions. If one parameter point fails a check the column is set to the following values for this point:

- `omega_c/T_c = -1`: The VEV configuration is not vanishing at  $T = 300$  GeV and therefore no SFOEWPT (in a single step) is possible.
- `omega_c/T_c = -2`: The next-to-leading order (NLO) VEV at zero temperature is not equal to the tree-level VEV, hence the parameter is not NLO stable and neglected.

- `omega_c/T_c=-3`: The parameter point provides electroweak VEV configurations above 255 GeV and is therefore neglected due to unphysical behaviour.<sup>6</sup>
- `omega_c/T_c=-4`: If the parameter point provides  $\omega_c/T_c < \text{C\_PT}$  the output is set to -4. Note that the default value of `C\_PT` is set to zero. In order to obtain in the output file only parameter points that provide an SFOEWPT, `C\_PT` has to be set to 1.
- `omega_c/T_c=-5`: The parameter point provides a vanishing or divergent VEV configuration at zero temperature and therefore the calculation is aborted.

If `omega_c/T_c > 0`, the parameter point has passed all tests. Note that for parameter points with an SFOEWPT the value has to be greater than one. Note, that the reason for errors can be multiple and be due to implementation errors or have a physics reason or both so that only the error itself will be reported.

#### 4.4.3 CalcCT

`CalcCT` is the executable for the calculation of the counterterms for a given parameter point. It is executed through the command line

##### CalcCT

```
./bin/CalcCT Model Inputfile Outputfile LineStart LineEnd
```

For each line, *i.e.* each parameter point, the various counterterms of the model are calculated. They are written out in the output file which contains a copy of the parameter point and appended to it in the same line the results for the counterterms. The first line of the output file contains the legend describing the entries of the various columns. An example call for the C2HDM would look like

```
1 ./bin/CalcCT c2hdm ../example/C2HDM_Input.dat output.csv 2 2
```

The output file `output.csv` should be the same as `example/C2HDM_Input.dat_CalcCT` up to numerical fluctuations.

#### 4.4.4 NLOVEV

`NLOVEV` is the executable calculating the global minimum of the loop-corrected effective potential at  $T = 0$  GeV for every point between the lines `LineStart` and `LineEnd` to be specified in the command line for the execution of the program:

##### NLOVEV

```
./bin/NLOVEV Model Inputfile Outputfile LineStart LineEnd
```

The output file contains the information on the parameter point for which the computed values at zero temperature of the NLO VEVs (in GeV) are appended in the same line, namely  $v(T = 0)$  and the individual VEVs  $\omega_k(T = 0) \equiv v_k$  ( $k = 1, \dots, n_v$ ), where  $n_v$  is the number the VEVs present in the investigated model. The first line of the output file again details the entries of the

<sup>6</sup>We chose the value of 255 GeV to account for potential fluctuations in the numerical result.

various columns. Note, that it can happen that the global minimum  $v(T = 0)$ , that is obtained from the NLO effective potential, is not equal to  $v = 246.22$  GeV any more. By writing out also  $v(T = 0)$  the user can check for this phenomenological constraint. An example call for the C2HDM would look like

```
1 ./bin/NLOVEV c2hdm ../example/C2HDM_Input.dat output.csv 2 2
```

The output file `output.csv` should be the same as `example/C2HDM_Input.dat_NLOVEV` up to numerical fluctuations.

#### 4.4.5 VEVEVO

VEVEVO provides the executable calculating the global minimum of the loop-corrected effective potential between the temperatures `TemperatureStart` and `TemperatureEnd`. The binary is called with

##### VEVEVO

```
./bin/VEVEVO Model Inputfile Outputfile Line TemperatureStart TemperatureStep TemperatureEnd
```

The output file contains the used parameter point extended with the values of the NLO VEVs at the given temperature. For each temperature step with a stepsize `TemperatureStep` a line is added to the output file. An example call for the C2HDM would look like

```
1 ./bin/VEVEVO c2hdm ../example/C2HDM_Input.dat output.csv 2 0 10 160
```

where the first data line of `C2HDM_Input.dat` would be used and the temperature would be varied from 0 GeV to 160 GeV with a stepsize of 10 GeV. The output file `output.csv` should be the same as `example/C2HDM_Input.dat_VEVEVO` up to numerical fluctuations.

#### 4.4.6 TripleHiggsCouplingsNLO

`TripleHiggsCouplingsNLO` is the executable of the program that calculates the triple Higgs couplings, derived from the third derivative of the potential with respect to the Higgs fields, for every point between the lines `LineStart` and `LineEnd` to be specified in the command line:

##### TripleHiggsCouplingsNLO

```
./bin/TripleHiggsNLO Model Inputfile Outputfile LineStart LineEnd
```

The output file contains the trilinear Higgs self-couplings derived from the tree-level potential, the counterterm potential and the Coleman-Weinberg potential at  $T = 0$  for all possible Higgs field combinations. The total NLO trilinear Higgs self-couplings are then given by the sum of these three contributions. The first line of the output file describes the entries of the various columns. An example call for the C2HDM would look like

```
1 ./bin/TripleHiggsNLO c2hdm ../example/C2HDM_Input.dat output.csv 2 2
```

The output file `output.csv` should be the same as `example/C2HDM_Input.dat_TripleHiggsNLO` up to numerical fluctuations.

#### 4.4.7 CalculateEWBG

CalculateEWBG is the executable of the program that calculates the BAU for each parameter point between *LineStart* and *LineEnd* in the different approaches. The command line reads:

#### CalculateEWBG

```
./bin/CalculateEWBG Model Inputfile Outputfile LineStart LineEnd EWBGConfigFile
```

So far, the routines for the calculation of the BAU are only implemented for the C2HDM. This means that at present *Model* can only be set to C2HDM. *EWBGConfigFile* allows to determine which approach is used for the calculation of the BAU. A sample config file is given in `BSMPT/example/EWBG_config.txt` and can be modified accordingly. The default config file has the following form

```
1   ### config file for the EWBG calculation (yes/no)
2
3   VIA Ansatz only including the top quark in the transport equations
4   Include:    yes
5
6   VIA Ansatz including the top and bottom quark in the transport equations
7   Include:    yes
8
9   VIA Ansatz including the top and bottom quark and the tau lepton in the
10  transport equations
11  Include:    yes
12
13  Via Ansatz treating the bottom quark massive
14  Massive:    yes
15
16  FH Ansatz with the plasma velocities
17  Include:    yes
18
19  FH Ansatz with the plasma velocities replaced through the second derivatives
20  Include:    no
21
```

By changing *yes/no* it is possible to switch on/off the different approaches in the calculation of the BAU. The spacing in front of *yes/no* has to be adhered to. The following approaches can be chosen:

- VIA approach with only the top quark included in the transport equations,
- VIA approach with top and bottom quarks included in the transport equations,
- VIA approach with top and bottom quarks and  $\tau$  lepton in the transport equations,
- VIA approach with the bottom quark treated massive (yes) or massless (no),
- FH approach with plasma velocities included,
- alternative FH approach with plasma velocities replaced using Eq. (43).

An example call for the C2HDM would look like

```
1 ./bin/CalculateEWBG c2hdm ../C2HDM_Input.dat output.csv 2 2 ../example/
  EWBG_config.txt
```

The output file `output.csv` should be the same as `example/C2HDM_Input.dat_EWBG` up to numerical fluctuations.

#### 4.4.8 PlotEWBG\_vw

The binary `PlotEWBG_vw` allows to calculate the BAU as a function of the bubble wall velocity  $v_W$ . Note that the wall velocity is treated as an additional input parameter in the implemented approaches. The binary is called by

##### PlotEWBG\_vw

```
./bin/PlotEWBG_vw Model Inputfile Outputfile Line vwMin vwStepsize vwMax EWBG-
ConfigFile
```

So far only the C2HDM is implemented so that *Model* has to be chosen accordingly. The line number *Line* determines the parameter point in the given input file. The BAU will be calculated for this parameter point for equidistant wall velocities between  $vwMin$  and  $vwMax$  with a stepsize of  $vwStepsize$ . `EWBGConfigFile` allows to specify which approach is used in the calculation. A sample config file can be found in `$BSMPT/example/EWBG_config.txt`. The options are the same as in the binary `CalculateEWBG`, cf. Sec. 4.4.7. An example call for the C2HDM would look like

```
1 ./bin/PlotEWBG_vw c2hdm ../example/C2HDM_Input.dat output.csv 2 0.05 0.01 0.15
  ../example/EWBG_config.txt
```

The output file `output.csv` should be the same as `example/C2HDM_Input.dat_PlotEWBG_vw` up to numerical fluctuations.

#### 4.4.9 PlotEWBG\_nL

The binary `PlotEWBG_nL` determines the left-handed fermion densities in front of the bubble wall as a function of the wall distance  $z$ . The binary is called by

##### PlotEWBG\_nL

```
./bin/PlotEWBG_nL Model Inputfile Outputfile Line vw EWBGConfigFile
```

We remind that at present *Model* can only be set to the C2HDM. The line number of the parameter point for which the calculation is performed is set by *Line*, and the input wall velocity  $v_W$  by *vw*. In `EWBGConfigFile` the user can choose which approach for the calculation of the BAU should be used, as explained in Sec. 4.4.7. A sample input file is provided in `$BSMPT/example/EWBG_config.txt`. In the output file for each step of the distance  $z$  an additional line is added with the corresponding results for the left-handed densities of the chosen approaches. An example call for the C2HDM would look like

```
1 ./bin/PlotEWBG_nL c2hdm ../example/C2HDM_Input.dat output.csv 2 0.1 ../example
  /EWBG_config.txt
```

The output file `output.csv` should be the same as `example/C2HDM_Input.dat_PlotEWBG_nL` up to numerical fluctuations.

## 5 Discussion of Approaches, Options and Approximations

We have implemented in `BSMPT v2` two different approaches for the formulation of the quantum transport equations, the `FH` approach and the `VIA` method, for which we also allow different options, *cf.* Sec. 4.4.7. We furthermore use various approximations. We plan to investigate in detail in a forthcoming publication the impact of the different approaches and approximations on the BAU. We discuss them more generally here in order to give some guidance to the user of the code.

### *The two different approaches for the computation of the BAU*

In the literature both the `FH` and the `VIA` method have been used to compute the BAU. Thus the BAU for the Minimal Supersymmetric Extension of the Standard Model (MSSM) has been obtained with the `VIA` method in [81] *e.g.*, and with the `FH` approach in [82–84]. While in both approaches the particle densities that contribute to the BAU are obtained from the Boltzmann equations, there is no agreement on their precise form. A systematic comparison of the two methods for the C2HDM is still missing. Ref. [85], where the quantum transport equations were derived from first principles in the Schwinger-Keldysh formalism, presents a brief general comparison with the `FH` and `VIA` approach mentioning also shortcomings inherent in each approach. Furthermore, a quantitative comparison between the different approaches is given for the MSSM. The author also points out that in the `VIA` method it is straightforward to include several flavours. In [50], a comparison was performed for a prototypical model of CP violation in the wall. In agreement with the results obtained for the MSSM, the authors found that the `VIA` estimate of the BAU is significantly larger. The authors of [50], who apply the `FH` approach to investigate the BAU, argue that these semiclassical results are more reliable. In view of missing further investigations we regard the question on which approach to be used as still an open issue and therefore offer both options in our code. We point out to the user, however, that in our experience the results obtained for the BAU in the `VIA` approach are considerably larger than those of the `FH` method, so that the computed BAU result should be rather regarded as an estimate and taken as an indication if the model under investigation might lead to sufficient BAU in principle.

### *Options provided for the two different approaches*

In the configuration file `EWGB_config.txt` presented in Sec. 4.4.7 different options can be chosen to compute the BAU. As stated in [85] the `VIA` approach can easily be extended to additional flavours. The first three options given in the configuration file allow in the `VIA` approach, in the order in which they appear, the inclusion of the top quark only, the additional inclusion of the bottom quark, and the inclusion of the top, bottom and tau. By choosing and comparing the different options the user can study the impact of additional flavours and get a feeling on possible directions for model building. The fourth option relates to the `VIA` approach in general. In case the bottom quark is included, its mass can be set to zero by setting the corresponding flag to 'no'. The last two options relate to two possible variants of the transport equations in the `FH` approach. In the first variant the plasma velocities are used, in the second they are expressed through derivatives, *cf.* Eq. (43). For a comparison of the two variants, see [86]. Offering the choice among these options allows the user to study the impact of the two approaches and, in the `VIA` approach, of the different fermion configurations. For the reasons stated above, we do not give a recommendation for which option to be used.

### *Small Wall Velocities*

As stated in Sec. 3.2 we apply the approximation of small wall velocities in the `FH` approach.

Recently, [50] rederived the fluid equations without making this approximation. It was found that the BAU suppression is a smooth function of the wall velocity and the sound speed barrier can safely be crossed. The authors furthermore pointed out some mistakes in the previous derivation of the FH approach. They presented also a numerical comparison of the BAU with their new results and their previous FH implementation. It is found that both results agree for small wall velocities. With increasing  $v_W$  they start to differ reaching a deviation below 30% for  $v_W = 0.1$  in the predicted BAU for the prototypical model studied in the paper. While the difference depends on the specific model, as a rough guideline we recommend not to use wall velocities above 0.1 when applying our code for the FH method. We will implement the new results of [50] which requires some major changes in the code in the next upgrades so that also larger wall velocities can be applied. In the meantime, the user can also study the effect of going slightly beyond 0.1. As long as the results for the BAU do not change drastically, the obtained numbers should still provide a reasonable estimate of the BAU. The VIA method does not utilize any explicit expansion in small  $v_W$ , it still assumes, however, small bubble wall dynamics in the derivation of the quantum transport equations. In this sense, we also advise the user to use bubble wall velocities of about the same magnitude as in the FH method.

#### *Impact of the wall profile*

As discussed in Sec. 3.1 we approximate the bubble wall profile by the kink profile, an approach that is frequently used in the literature. We also described in Sec. 3.1 how we obtain the barrier height. We furthermore varied the wall thickness for specific benchmark points and found that the impact on the BAU was in the percentage region. In order to estimate the error made by our approximation of the wall profile we would need to compare it with the bounce solution.

#### *Usage of the critical temperature*

In `BSMPT v2` we are not able to estimate the nucleation temperature  $T_N$  and the bounce solution. Instead we determine the wall thickness and bubble profile at the critical temperature. One could argue to provide the possibility to use the nucleation temperature obtained by a different code. We deliberately refrain, however, from including the nucleation temperature from a different code. The reason is that this would be inconsistent. Changing the temperature from the critical to the nucleation temperature would yield a different vacuum structure of the potential. The new vacuum structure would prevent the usage of the `BSMPT` algorithms, since these require the degenerate vacua at the critical transition point. Remark that we define and apply the  $VEV(s)$  determined at the critical temperature. In other words, the results obtained with  $T_N$  instead of  $T_c$  would imply inconsistent solutions. We therefore do not provide the option to use  $T_N$  obtained from a different code. The consistent solution requires the future determination of  $T_N$  and the bounce solution within `BSMPT`. An approximate feeling of the influence of our approximation can be obtained by investigating the resulting BAU for given  $\xi_c$  values in the model under investigation (at present only the C2HDM is possible) in a large number of allowed parameter points of the model. This requires a large scan and a detailed phenomenological investigation that we plan to perform in a forthcoming paper.

## 6 How to add a New Model

In the following section a description is given on how to add a new model to the `BSMPT` framework. A template class is provided to simplify the implementation. For the definition of the tensors derived from the Lagrangian in the gauge basis, we refer to the previous version of the manual [21] and focus here on the differences between the two versions. In the following, we give the steps

to be performed to to modify the class template to the desired model referred to as `YourModel`. The concrete implementation of a toy model will be given in Sec. 6.1.

For the inclusion of a new model, the following steps have to be performed:

- 1) The class template header file in

`$BSMPT/include/BSMPT/models/ClassTemplate.h`

is copied to

`$BSMPT/include/BSMPT/models/YourModel.h`

In this header file all occurrences of `Class_Template` have to be changed to `YourModel`.

- 2) To call the correct model in the binaries the model ID has to be provided. `YourModelID` has to be added as an enum in

`$BSMPT/include/BSMPT/models/IncludeAllModels.h`

below the already provided models *e.g.* like

```
1 enum class ModelIDs
2 {
3     ...
4     YourModelID,
5     ...
6     // DO NOT EDIT the part below
7     stop
8 };
```

Right below in `ModelNames`, a new entry for the new model is to be added through

```
1 const std::unordered_map<std::string, ModelIDs> ModelNames{
2     ...
3     {"modelname" , ModelIDs::YourModelID},
4     ...
5 };
```

Note that `modelname` has to be in lowercase and will be used to call the model in the binaries.

- 3) In the file

`$BSMPT/src/models/IncludeAllModels.cpp`

the header for the new model has to be added via the additional include

```
1 #include <BSMPT/models/YourModel.h>
```

Afterwards the function `FChoose` have to be extended by the additional switch statement

```

1 std::unique_ptr<Class_Potential_Origin> FChoose(ModelIDs choice){
2 using namespace Models;
3 switch (choice) {
4 ...
5 case ModelIDs::YourModelID :return std::make_unique<YourModel>();break;
6 ...
7 }
8 }

```

#### 4) The template

\$BSMPT/src/models/ClassTemplate.cpp

has to be copied to

\$BSMPT/src/models/YourModel.cpp

and changed accordingly. All occurrences of `Class_Template` have to be changed to `YourModel`. We provide comments in the class templates indicating what else needs to be changed. The definition of the tensor structure can be found in [21]. The following functions have to be adapted for the new model:

```

Class_Template
ReadAndSet
addLegendCT
addLegendTemp
addLegendTripleCouplings
addLegendVEV
set_gen
set_CT_Pot_Par
write
TripleHiggsCouplings
calc_CT
SetCurvatureArrays
CalculateDebyeSimplified
VTreeSimplified
VCounterSimplified
Debugging7

```

#### 5) As last step the model has to be added to the `cmake` file. In

\$BSMPT/src/models/CMakeLists.txt

---

<sup>7</sup>In fact, the function `Debugging` is only used by the Test executable and is provided only for the user to perform some checks.

the additional include has to be added

```
1 #{header_path}/YourModel.h
```

and the file `YourModel.cpp` has to be linked by adding

```
1 set(src  
2 ...  
3 YourModel.cpp  
4 ...  
5 )
```

After performing these steps and rebuilding the program by following the steps described in Sec. 4.3 `YourModel` should compile. The concrete implementation of the model parameters is described in the following section by considering a simple toy model. The corresponding tensors are defined in [21].

## 6.1 Toy Model Example

As example we take a model with one scalar particle  $\phi$  which develops a VEV  $v$ , couples to one fermion  $t$  with the Yukawa coupling  $y_t$ , and to one gauge boson  $A$  with the gauge coupling  $g$ . The relevant pieces of the Lagrangian are given by ( $\Phi = \phi + v$ )

$$-\mathcal{L}_S = \frac{m^2}{2} (\phi + v)^2 + \frac{\lambda}{4!} (\phi + v)^4 \quad (76a)$$

$$-\mathcal{L}_F = y_t t_L t_R (\phi + v) \quad (76b)$$

$$\mathcal{L}_G = g^2 A^2 (\phi + v)^2 . \quad (76c)$$

We therefore have  $i, j, k, l = 1, I, J = 1, 2, a, b = 1$  for the tensors defined in [21]. Here  $I, J = 1, 2$  corresponds to  $t_L$  and  $t_R$ , the left- and right-handed projections of the fermion  $t$ . The tensors are given by

$$L^i = \partial_v (-\mathcal{L}_S)|_{\phi=0, v=0} = 0 \quad (77a)$$

$$L^{ij} = \partial_v^2 (-\mathcal{L}_S)|_{\phi=0, v=0} = m^2 \quad (77b)$$

$$L^{ijk} = \partial_v^3 (-\mathcal{L}_S)|_{\phi=0, v=0} = 0 \quad (77c)$$

$$L^{ijkl} = \partial_v^4 (-\mathcal{L}_S)|_{\phi=0, v=0} = \lambda \quad (77d)$$

$$Y^{IJK} = \begin{cases} 0 & I = J \text{ (} I, J = t_L, t_R \text{)} \\ y_t & I \neq J \text{ (} I, J = t_L, t_R \text{)} \end{cases} \quad (77e)$$

$$G^{abij} = \partial_A^2 \partial_v^2 (\mathcal{L}_G) = 4g^2 . \quad (77f)$$

The counterterm potential reads

$$V^{\text{CT}} = \frac{\delta m^2}{2} (\phi + v)^2 + \frac{\delta \lambda}{4!} (\phi + v)^4 + \delta T (\phi + v) . \quad (78)$$

The renormalisation conditions yield the following relations for the counterterms

$$\delta T + v \delta m^2 + \frac{1}{6} v^3 \delta \lambda = - \partial_\phi V^{\text{CW}}|_{\phi=0} \quad (79a)$$

$$\delta m^2 + \frac{v^2}{2} \delta \lambda = - \partial_\phi^2 V^{\text{CW}}|_{\phi=0} . \quad (79b)$$

The resulting system of equations is overconstrained. The tadpole counterterm is chosen to be arbitrary as

$$\delta T = t, \quad \text{with } t \in \mathbb{R}, \quad (80)$$

yielding the remaining counterterms as

$$\delta\lambda = \frac{3t}{v^3} + \frac{3}{v^3} \left( \partial_\phi V^{\text{CW}}|_{\phi=0} \right) - \frac{3}{v^2} \left( \partial_\phi^2 V^{\text{CW}}|_{\phi=0} \right) \quad (81a)$$

$$\delta m^2 = -\frac{3}{2v} \left( \partial_\phi V^{\text{CW}}|_{\phi=0} \right) + \frac{1}{2} \left( \partial_\phi^2 V^{\text{CW}}|_{\phi=0} \right) - \frac{3t}{2v}. \quad (81b)$$

In the following we will discuss the additional steps needed for the implementation of this concrete toy model.

### 6.1.1 Proper Link of the Model

As a first step we follow the steps described at the beginning of Sec. 6. The corresponding model ID `ToyModel` and model name `toymodel` are added to `IncludeAllModels.h` and `IncludeAllModels.cpp`, respectively. For the model header file `ToyModel.h` and the `ToyModel.cpp` file the template class files can be used, where the occurrences of `ClassTemplate` have to be changed accordingly. When the steps 1-5 described at the beginning of Sec. 6 are complete some additional information is needed. In the header file `ToyModel.h` the variables for the potential and for the remaining Higgs coupling parameters as well as for the counterterm constants have to be added by including

```
1 double ms, lambda, dms, dlambd, dT, yt, g;
```

Here `ms` denotes the mass parameter squared,  $m^2$ , and `dms`, `dlambd` are the counterterms  $\delta m^2$ ,  $\delta\lambda$ . Note that the parameters do not need to be set yet, they are only declared here.

### 6.1.2 ToyModel.cpp

In this section, we will briefly discuss which essential adaptations in `ToyModel.cpp` are needed to implement a working model into `BSMPT v2`. The user is further guided by comments in the template source code.

**Toy\_Model()** The numbers of Higgs particles, potential parameters, counterterms and VEVs have to be specified in the constructor `Toy_Model()` and the variable 'Model' has to be set to the selected model. For the toy model example, this corresponds to

```
1 Toy_Model::Toy_Model(){
2   Model = ModelID::ModelIDs::TOYMODEL;
3   NNeutralHiggs = 1; // Number of neutral Higgs bosons
4   NChargedHiggs = 0; // Number of charged Higgs bosons
5   nPar          = 2; // Number of independent input parameters
6   nParCT       = 3; // Number of counterterms
7   nVEV         = 1; // Number of non-zero VEVs
8   NHiggs       = NNeutralHiggs+NChargedHiggs;
9   VevOrder.resize(nVEV);
10  VevOrder[0] = 0;
11  UseVTreeSimplified = false; // Option for using a simplified tree-level
   potential-> false uses the generic implementation
12  UseVCounterSimplified = false; // Option for using a simplified counterterm
   potential-> false uses the generic implementation
13 }
```

It should be emphasized that internally the Higgs potential is built by the vector of the Higgs field containing all fields, with a length of `NHiggs`. For the toy model this vector would have only one component  $\phi$ . For a more complex model this might not be the case. However, not all field components need to have a non-zero VEV. In this case, in order to determine which field components should be taken into account in the minimisation of the potential, the vector `VevOrder` has to specify which field components of the vector with length `NHiggs` have a VEV. The code

```
1 VevOrder[0] = 0;
```

would attribute a VEV to the first component of the field vector. For instance, our implementation of the CxSM has the following constructor

```
1 Class_CxSM::Class_CxSM()
2 {
3   Model = ModelID::ModelIDs::CXSM;
4   NNeutralHiggs = 4; // Number of neutral Higgs bosons at T = 0
5   NChargedHiggs=2; // Number of charged Higgs bosons at T = 0 (all d.o.f.)
6   nPar = 10+3; // Number of parameters in the tree-level Lagrangian
7   nParCT = 9+6; // Number of parameters in the counterterm potential
8
9   nVEV=3; // Number of VEVs to minimize the potential
10  NHiggs = NNeutralHiggs+NChargedHiggs;
11
12  VevOrder.resize(nVEV);
13  VevOrder[0] = 3;
14  VevOrder[1] = 4;
15  VevOrder[2] = 5;
16
17  UseVTreeSimplified = false;
18  UseVCounterSimplified = false;
19 }
```

implying that the Higgs field vector has fields with VEVs at the positions 3,4 and 5. The resulting three-dimensional vector containing all field components with a VEV of the CxSM corresponds then to the vacuum structure of the given model.

**Input Read-in** BSMPT v2 reads the input through `std::stringstream` where each parameter point is given as a simple line with tab separation. The user has to specify the order of the respective input parameters in the function `ReadAndSet()`. For the toy model under consideration two input parameters,  $m^2$  and  $\lambda$ , have to be specified

```
1 void Toy_Model::ReadAndSet(const std::string& linestr, std::vector<double>& par
2 )
3 {
4   std::stringstream ss(linestr);
5   double tmp;
6   double lms, llambda;
7   for(int k=1;k<=2;k++)
8   {
9     ss>>tmp;
10    if(k==1) lms = tmp; // Class member lms is set to the respective input
11    parameter
12    else if(k==2) llambda = tmp; //Class member llambda is set to the
13    respective input parameter
14  }
15  par[0] = lms;
```

```

13  par[1] = llambda;
14  set_gen(par); // Setting of all model parameters with the given input
      parameters par
15  return ;
16 }

```

where `par` contains all input parameters in a fixed order. The function `set_gen` sets all remaining model parameters in accordance with the input parameters. This function has changed with respect to the previous BSMPT version and old files have to be adapted for compatibility with BSMPT v2.

`set_gen()` This function allows to express all model parameters in accordance with the input parameters. This function is called in the `ReadAndSet()` function after the input parameter vector `par` is set. Further SM input parameters are provided by

`$BSMPT/include/BSMPT/models/SMparam.h`

and can be used to set up the parameters of the toy model. For the toy model, the `set_gen` function would look like

```

1 void Toy_Model::set_gen(const std::vector<double>& par) {
2   ms = par[0]; //Class member is set in accordance with the input parameters
3   lambda = par[1]; //Class member is set in accordance with to the input
      parameters
4   g=C_g; //SM SU(2) gauge coupling --> SMparam.h
5   yt = std::sqrt(2)/C_vev0 * C_MassTop; //Top Yukawa coupling --> SMparam.h
6   scale = C_vev0; //Renormalisation scale is set to the SM VEV
7   vevTreeMin.resize(nVEV);
8   vevTree.resize(NHiggs);
9   vevTreeMin[0] = C_vev0;
10  vevTree=MinimizeOrderVEV(vevTreeMin);
11  if(!SetCurvatureDone) SetCurvatureArrays();
12 }

```

More complex models might require to set further parameters of the Lagrangian. The analytic formulas expressing these parameters in terms of the input parameters can be implemented in `set_gen`.

`SetCurvatureArrays()` The tensors of the Lagrangian of the new model have to be implemented in the function `SetCurvatureArrays()`. The notation follows the definition in [21] and the corresponding variable names are given by

$$\text{Curvature\_Higgs\_L1}[i] \hat{=} L^i \quad (82a)$$

$$\text{Curvature\_Higgs\_L2}[i][j] \hat{=} L^{ij} \quad (82b)$$

$$\text{Curvature\_Higgs\_L3}[i][j][k] \hat{=} L^{ijk} \quad (82c)$$

$$\text{Curvature\_Higgs\_L4}[i][j][k][l] \hat{=} L^{ijkl} \quad (82d)$$

$$\text{Curvature\_Gauge\_G2H2}[a][b][i][j] \hat{=} G^{abij} \quad (82e)$$

$$\text{Curvature\_Quark\_F2H1}[I][J][k] \hat{=} Y^{IJK}. \quad (82f)$$

Technically, it is possible to use `Curvature_Quark_F2H1` to store all quarks and leptons simultaneously, but as they do not mix the program provides besides `Curvature_Quark_F2H1` where

$I, J$  run over all quarks, also the structure `Curvature_Lepton_F2H1[I][J][k]` where  $I, J$  run over all leptons. Only non-zero tensor coefficients need to be provided. The implementation for the toy model would look like

```

1 void Toy_Model::SetCurvatureArrays(){
2   initVectors();
3   SetCurvatureDone=true;
4   for(size_t i=0;i<NHiggs;i++) HiggsVev[i] = vevTree[i];
5   Curvature_Higgs_L2[0][0] = ms;
6   Curvature_Higgs_L4[0][0][0][0] = lambda;
7   Curvature_Gauge_G2H2[0][0][0][0] = 4*std::pow(g,2);
8   Curvature_Quark_F2H1[1][0][0] = yt;
9   Curvature_Quark_F2H1[0][1][0] = yt;
10 }

```

`set_CT_Pot_Par()` Analogously, the curvature terms for the counterterm potential have to be set. The corresponding tensors are defined as in the tree-level potential with the additional suffix `_CT_`. For the toy model the implementation would look like

```

1 void Toy_Model::set_CT_Pot_Par(const std::vector<double>& par){
2
3   dT = par[0];
4   dlambda = par[1];
5   dms = par[2];
6
7   Curvature_Higgs_CT_L1[0] = dT;
8   Curvature_Higgs_CT_L2[0][0] = dms;
9   Curvature_Higgs_CT_L4[0][0][0][0] = dlambda;
10 }

```

`calc_CT()` The counterterms are computed numerically in the function `calc_CT()`. To do so, the user has to implement the formulae for the counterterms that were derived beforehand analytically in terms of the derivatives of the Coleman-Weinberg potential, *cf.* Eqs. (80), (81a) and (81b) for our template model. The derivatives of  $V^{CW}$  are provided by the program through the function calls `WeinbergFirstDerivative` and `WeinbergSecondDerivative`.

```

1 std::vector<double> Toy_Model::calc_CT() const {
2   std::vector<double> parCT;
3   ...
4   std::vector<double> WeinbergNabla,WeinbergHesse;
5   WeinbergNabla = WeinbergFirstDerivative(); //Call for the calculation of the
6   first derivative of the Coleman-Weinberg potential
7   WeinbergHesse = WeinbergSecondDerivative();//Call for the calculation of the
8   second derivative of the Coleman-Weinberg potential
9   ...
10  double t = 0;
11  parCT.push_back(t); // Tadpole counterterm dT
12  parCT.push_back(3.0*t/std::pow(C_vev0,3) + 3.0/std::pow(C_vev0,3) *
13  NablaWeinberg(0) -3.0/std::pow(C_vev0,2) *HesseWeinberg(0,0)); // Analytic
14  formula of the counterterm dlambda
15  parCT.push_back(-3.0/(2*std::pow(C_vev0,2)) *NablaWeinberg(0) + 1.0/2.0 *
16  HesseWeinberg(0,0) -3.0*t/(2*C_vev0)); // Analytic formula of the
17  counterterm dms
18  return parCT;
19 }

```

The remaining code base (indicated by '...') can be copied from the template class file.

**TripleHiggsCouplings()** This function provides the trilinear loop-corrected Higgs self-couplings as obtained from the effective potential. They are calculated from the third derivative of the Higgs potential with respect to the Higgs fields in the gauge basis and then rotated to the mass basis. The scalar mass matrix is built from all the scalar degrees of freedom of the theory, which we refer to as the gauge basis [21]. Since the numerical routines in **Eigen** return the mass eigenvalues ordered by ascending masses, the corresponding eigenstates have to be identified with the respective Higgs bosons. Therefore, it is necessary to map both bases, the mass ordered mass eigenstate basis and the physical Higgs boson basis. The mapping is achieved through the vector **HiggsOrder(NHiggs)** *e.g.*

```
1 for(size_t i=0;i<NHiggs;i++) HiggsOrder[i]=value[i];
```

The mapping **value** is defined by the user according to the ordering that is desired in the Higgs basis. Thus **HiggsOrder[0] = 5** *e.g.* would assign the 6th lightest particle to the first position. The particles can be selected through the mixing matrix elements.

All following functions add specific legends to the output header.

**addLegendTripleCouplings()** The function **addLegendTripleCouplings** extends the legend by the column names for the trilinear Higgs couplings derived from the tree-level, the counterterm and the Coleman-Weinberg potential. In order to do so, the user first has to make sure to define the names of the Higgs particles of the model in the vector **particles**. In the toy model only one Higgs boson is present, which we refer to as  $H$  and hence set

```
1 particles[0] = "H";
```

**addLegendTemp()** In this function, the column names for  $T_c$ ,  $v_c$  and the VEVs are added to the legend. The order should be  $T_c$ ,  $v_c$  and then the names of the individual VEVs. These VEVs have to be added in the same order as given in the function **MinimizeOrderVEV**.

**addLegendVEV()** This function adds the column names for the VEVs that are given out. The order has to be the same as given in the function **MinimizeOrderVEV**.

**addLegendCT()** In this function, the legend for the counterterms is added. The order of the counterterms has to be the same as the one set in the function **set\_CT\_Pot\_Par(par)**.

**VTreeSimplified, VCounterSimplified** The functions

```
1 VTreeSimplified(const std::vector<double>& v)
2 VCounterSimplified(const std::vector<double>& v)
```

can be used to explicitly implement the formulas for the tree-level and counterterm potential in terms of the classical fields  $\omega$ , in our example these are Eqs. (76a) and Eq. (78), respectively, with  $\phi = 0$  and  $v \equiv \omega$ . Implementing these may improve the runtime of the programs. An example is given in the template class.

**write()** The function `write()` allows us to print all needed parameters in the terminal and might be used for the debugging procedure or some investigation of parameter behaviour. One minimalist example for the toy model could look like

```

1 void Class_Template::write() const {
2
3     std::cout << "The parameters are : " << std::endl;
4     std::cout << "lambda = " << lambda << std::endl
5         << "m^2 = " << ms << std::endl;
6
7     std::cout << "The counterterm parameters are : " << std::endl;
8     std::cout << "dT = " << dT << std::endl
9         << "dlambda = " << dlambda << std::endl
10        << "dm^2 = " << dms << std::endl;
11     std::cout << "Some interesting number" << lambda * ms << std::endl;
12 }

```

## 7 Using BSMPT as a library

During the installation, BSMPT v2 is exported as a `cmake` package. It is possible to link BSMPT v2 in an existing `cmake` project by including the line

```
1 find_package(BSMPT 2.0)
```

which provides the `BSMPT::Models`, `BSMPT::Minimizer`, `BSMPT::ThermalFunctions` and `BSMPT::Utility` modules. Furthermore, the modules `BSMPT::Baryo`, `BSMPT::LibWallThickness` and `BSMPT::Kfactors` are available if the boost library is provided.

## 8 Upgrading from BSMPT v1.x to v2

With the upgrade from v1 to v2 the interface to the basic functions and most of the return types of the functions have changed. Private implementations for BSMPT have to be adapted to be compatible with BSMPT v2. It is recommended to use the template class for new model implementations. If there are remaining compatibility problems, contact us either through github or via mail [bsmpt@lists.kit.edu](mailto:bsmpt@lists.kit.edu).

## 9 Conclusions

We have presented the C++ code BSMPT v2, an extension of the previous code BSMPT that calculates the strength of the electroweak phase transition in Higgs sector extensions beyond the SM. The main new feature is the implementation of the calculation of the BAU in two different approximations, the FH and the VIA approach. Presently, this is applicable for the C2HDM and will be extended to include further models in future upgrades of the code. Furthermore, a new model, the CxSM has been included. We also added the possibility to change the renormalisation scale in the computation of the loop-corrected effective potential. The newly implemented model CxSM, the computation of the BAU in the two approaches FH and VIA and the additional changes and new features have been presented in detail along with a description of the procedure for the implementation of new models. This has been changed as well with respect to the previous version of BSMPT. The code can be downloaded at the url: <https://github.com/phbasler/BSMPT>.

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## Appendix

### A Tadpole Equations for the CxSM

The local minima of the tree-level potential of Eq. (1) are given by

$$0 = \frac{\partial V}{\partial \Phi^\dagger} \quad (83)$$

$$0 = \frac{\partial V}{\partial S^\dagger} . \quad (84)$$

This yields the following three equations

$$0 = \frac{v}{4} (v^2 \lambda + \delta_2 v_a^2 + \delta_2 v_s^2 + 2m^2) \quad (85a)$$

$$0 = \text{Re}(a_1) \sqrt{2} - \frac{\text{Im}(b_1)}{2} v_a + \frac{v_s}{4} (d_2 v_a^2 + d_2 v_s^2 + \delta_2 v^2 + 2\text{Re}(b_1) + 2b_2) \quad (85b)$$

$$\text{Im}(a_1) \sqrt{2} + \text{Im}(b_1) \frac{v_s}{2} = \frac{v_a}{4} (d_2 v_a^2 + d_2 v_s^2 + \delta_2 v^2 - 2\text{Re}(b_1) + 2b_2) . \quad (85c)$$

For the different vacuum configurations they are solved for different parameters. The solutions are

**Case  $v_s \neq 0 \wedge v_a \neq 0$**

$$\text{Re}(a_1) = \frac{\sqrt{2} d_2}{4} v_s (v_s^2 + v_a^2) - \frac{\sqrt{2} \delta_2}{4} v_s v^2 + \text{Im}(a_1) \frac{v_s}{v_a} + \frac{\sqrt{2} \text{Im}(b_1)}{4} \left( v_a + \frac{v_s^2}{v_a} \right) - \frac{b_2 v_s}{\sqrt{2}} \quad (86a)$$

$$\text{Re}(b_1) = b_2 + \frac{d_2}{2} (v_s^2 + v_a^2) + \frac{\delta_2}{2} v^2 - \frac{2\sqrt{2} \text{Im}(a_1)}{v_a} - \text{Im}(b_1) \frac{v_s}{v_a} \quad (86b)$$

$$m^2 = -\frac{\delta_2}{2} (v_s^2 + v_a^2) - \frac{\lambda}{2} v^2 . \quad (86c)$$

**Case  $v_s \neq 0 \wedge v_a = 0$**

$$\text{Im}(a_1) = -\frac{\sqrt{2}}{4} \text{Im}(b_1) v_s \quad (87a)$$

$$\text{Re}(b_1) = -b_2 - \frac{d_2 v_s^2}{2} - \frac{\delta_2 v^2}{2} - \frac{2\sqrt{2} \text{Re}(a_1)}{v_s} \quad (87b)$$

$$m^2 = -\frac{\delta_2 v_s^2}{2} - \frac{\lambda v^2}{2} . \quad (87c)$$

Case  $v_s = 0 \wedge v_a \neq 0$

$$\text{Re}(a_1) = \frac{\sqrt{2}}{4} \text{Im}(b_1) v_a \quad (88a)$$

$$\text{Re}(b_1) = b_2 + \frac{d_2 v_a^2}{2} + \frac{\delta_2 v^2}{2} - \frac{2\sqrt{2} \text{Im}(a_1)}{v_a} \quad (88b)$$

$$m^2 = -\frac{\delta_2 v_a^2}{2} - \frac{\lambda v^2}{2}. \quad (88c)$$

Case  $v_s = 0 \wedge v_a = 0$

$$\text{Im}(a_1) = 0 \quad (89a)$$

$$\text{Re}(a_1) = 0 \quad (89b)$$

$$m^2 = -\lambda \frac{v^2}{2}. \quad (89c)$$

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