
Exploring the Limits of the WIMP
Paradigm

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Artificial Intelligence (AI) has been used during the making of this thesis to support the grammar and style of the text. ChatGPT¹ has been used throughout the thesis to assist with spelling and grammar, as well as to paraphrase selected sentences for improved clarity and conciseness. All suggested changes were carefully reviewed before incorporation.

Furthermore, ChatGPT and Claude² have been used in Python code generation to help in plotting results and fixing bugs in C++. All proposed changes were checked and tested to ensure factual correctness. No generative AI tools have been used to derive or evaluate any of the results presented in this thesis.

¹Conversational AI model of OpenAI, <https://chatgpt.com/> (Access: August 31, 2026)

²Constitutinal AI model of Antrophic, <https://claude.ai/> (Access: August 31, 2026)

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**”Ihr wollt meinen Schatz? Den könnt ihr haben!
Sucht ihn doch! Irgendwo hab ich den größten
Schatz der Welt versteckt!” - Gol D. Roger**

Abstract

Weakly-Interacting-Massive-Particles (WIMP) provide a possible solution to the unanswered question of the underlying nature of dark matter in the universe. In this thesis, we explore the WIMP paradigm with different theoretical frameworks in order to get a deeper understanding of dark matter observables, which can be tested in current and future experiments.

In order to gain further insight into the impact of experimental constraints on parameter scans and their interplay with each other, we investigate the complex Two-Higgs Doublet model. Here, we quantify the allowed CP-violation in the fermionic couplings to the Standard Model-like Higgs boson. To improve our scanning procedure, we furthermore employ modern machine learning algorithms.

Exploring the parameter space of the Next-to-Minimal Supersymmetric Standard Model can become a tedious task, due to the large number of parameters in the model. We therefore develop the tool **NMSSMScanner**, which allows us to explore the parameter space in a convenient way. As a proof-of-concept, we maximize the production cross section of a resonant non-Standard Model-like Higgs boson decaying into various final states. Furthermore, we calculate the dark matter relic density and direct detection cross section in this model to further constrain the available parameter space with experimental data. To incorporate these features into our toolchain, the dark matter code **RelExt** is extended by an implementation of the calculation of the relic abundance and the direct detection cross section in this theoretical framework.

In addition, we calculate the dark matter relic density at next-to-leading order including electroweak and QCD corrections in the framework of the Complex Singlet Extension of the Standard Model. We argue that the inclusion of higher-order calculations is important in understanding the parameter space in dark matter models. This work is used as a proof-of-concept, in order to automate the next-to-leading order relic density calculation in **RelExt** for arbitrary models in future works.

Zusammenfassung

Schwach wechselwirkende massive Teilchen (*engl. weakly interacting massive particles (WIMP)*) können eine mögliche Antwort auf die Frage nach der zugrunde liegenden Natur von dunkler Materie darstellen. In dieser Arbeit werden wir das sogenannte WIMP-Paradigma in verschiedenen theoretischen Modellen untersuchen, um ein tieferes Verständnis der Observablen des dunklen Materieteilchens zu gewinnen. Diese können in gegenwärtigen und zukünftigen Experimenten getestet werden.

Um weiterführende Einblicke in die Auswirkungen experimenteller Einschränkungen auf Scans im Parameterbereich und das Zusammenspiel der Parameter zu erhalten, werden wir das komplexe Zwei-Higgs-Dublett-Modell untersuchen. Hierbei werden wir die theoretisch erlaubte Ladungs- und Paritätsverletzung in den fermionischen Kopplungen zum Standardmodell-Higgsteilchen quantifizieren. Dabei werden wir moderne Machine-Learning-Algorithmen zur Verbesserung unserer Scanverfahren einsetzen.

Die Untersuchung des nichtminimalen supersymmetrischen Standardmodells kann aufgrund der großen Anzahl an Parametern zu einer mühsamen Aufgabe werden. Wir entwickeln deshalb ein Tool, mit dem man den Parameterraum bequem untersuchen kann. Als Proof-of-Concept wird der Wirkungsquerschnitt für die resonante Produktion eines nicht im Standardmodell enthaltenen Higgsbosons maximiert, welches in verschiedene Endzustände zerfällt.

Des Weiteren berechnen wir in diesem Modell die Reliktdichte der dunklen Materie sowie den Wirkungsquerschnitt für den direkten Nachweis von dunklen Materieteilchen in Streuexperimenten. Hierfür wird der Code `RelExt` erweitert, indem die Berechnung der Reliktdichte und des Wirkungsquerschnittes für die dunkle-Materie-Streuung an Nukleonen implementiert wird.

Darüber hinaus wird die Reliktdichte im Kontext der komplexen Singulett-Erweiterung des Standardmodells auf nächsthöherer Ordnung berechnet. Dabei wird gezeigt, dass die Hinzunahme von Korrekturen höherer Ordnung wichtig ist, um den Parameterbereich von Dunkle-Materie-Modellen besser zu verstehen. Diese Arbeit wird als Proof-of-Concept dienen, um in zukünftigen Arbeiten die Berechnung der Reliktdichte auf nächsthöherer Ordnung für beliebige Modelle in `RelExt` zu automatisieren.

List of Publications

The work presented in this thesis is based in part on the following articles (published or under review).

1. R. Boto, T. N. Dao, F. Egle, K. Elyaouti, M. Gabelmann, M. Mühlleitner, J. Plotnikov, *NMSSMScanner: Efficient Scans in the NMSSM Parameter Space Proof of Concept*, arXiv:2604.25009 [hep-ph]
2. R. Boto, K. Elyaouti, D. Fontes, M. Gonçalves, M. Mühlleitner, J. C. Romão, R. Santos, J. P. Silva, *Reassessing CP Violation in the C2HDM with Machine Learning*, arXiv:2601.15227 [hep-ph]
3. R. Capucha, K. Elyaouti, M. Mühlleitner, J. Plotnikov, R. Santos, *RelExt: A New Dark Matter Tool for the Exploration of Dark Matter Models*, Comput. Phys. Commun. **320** (2026) 109968. doi:10.1016/j.cpc.2025.109968, arXiv:2503.13087 [hep-ph]
4. P. Brica, K. Elyaouti, P. Gabriel, M. Mühlleitner, R. Santos, *Full Next-To Leading-Order Electroweak and QCD Corrections to the Relic Density in the CxSM*, arXiv:2607.19179 [hep-ph]

Publications that are not Presented in this Thesis

- R. Capucha, K. Elyaouti, M. Mühlleitner, J. Plotnikov, R. Santos, *Freeze-in as a Complementary Process to Freeze-Out*, JHEP **09** (2024) 113. doi:10.1007/JHEP09(2024)113, arXiv:2407.04809 [hep-ph]

Contents

1. Introduction	1
I. Theoretical Overview	5
2. Theories Beyond the Standard Model	7
2.1. Standard Model of Particle Physics	7
2.1.1. The Higgs Mechanism	8
2.1.2. Yukawa Sector	10
2.2. Complex Singlet Extension of the Standard Model	12
2.3. The Complex Two-Higgs-Doublet-Model	13
2.4. Next-to-Minimal Supersymmetric Standard Model	16
3. Brief Overview of the Standard Model of Cosmology	21
3.1. General Relativity	21
3.2. Friedmann-Lemaître-Robertson-Walker Metric and the Friedmann Equations	22
3.3. Energy Budget of the Universe	22
3.4. Cosmic Microwave Background	23
3.5. Computation of the Dark Matter Relic Density	25
3.6. Direct Detection	30
II. Investigation of CP-Violation in the Complex Two-Higgs-Doublet Model	35
4. Introduction	37
4.1. Electron Electric Dipole Moment	38
5. Numerical Setup of the Analysis	47
5.1. Experimental and Theoretical Constraints	47
5.1.1. Theoretical Constraints	47
5.2. Experimental Constraints	48
5.3. Scan Ranges	49
6. Phenomenology with Strategy 1	51
6.1. Results	51
7. Phenomenology with Machine Learning Algorithms	53
7.1. Covariant Matrix Adaptation Evolutionary Strategy	54
7.2. Histogram Based Outlier System	54
7.3. Phenomenology with Strategy 2	55
8. Conclusion	59
III. Dark Matter Analysis in the NMSSM	61
9. Introduction	63
9.1. Dark Matter Relic Density in the NMSSM	64
9.1.1. Thermally Averaged Cross Section	66

9.2. Direct Detection in the NMSSM	68
10. RelExt - A Dark Matter Tool for Efficient Scans	71
10.1. New Model Implementation	72
10.2. DM Observables	77
11. Numerical Analysis	81
11.1. Organization of the Scan	81
11.2. Parameter Ranges	83
11.3. Scan Procedure	84
12. Results	85
13. Conclusion	93
 IV. The Dark Matter Relic Density at Next-to-Leading Order	 95
14. Introduction	97
14.1. Relic Density at Next-to-Leading Order	98
15. Renormalization and the Treatment of Infrared Divergences in the CxSM	101
15.1. On-Shell Renormalization	102
15.2. Scalar Sector	102
15.3. Electroweak and Fermionic Sector	107
15.4. Parameter Conversion between Renormalization Schemes	109
15.5. Infrared Divergences	109
15.5.1. Phase Spaces	110
15.5.2. Catani-Seymour Subtraction Method	113
16. Numerical Analysis	117
16.1. Theoretical Constraints	117
16.2. Experimental Constraints	118
16.3. Parameter Scan	118
17. Results	121
17.1. Relative Correction to the Dark Matter Relic Abundance	121
17.2. Impact of the QCD Corrections on the Relic abundance	122
17.3. Impact of Electroweak and QCD Corrections on the Relic Abundance	124
18. Conclusion	129
 V. Conclusion and Overview	 131
 19. Final Conclusion and Outlook	 133
 A. Relevant Couplings for the Direct Detection Calculation in the NMSSM	 135
A.1. Higgs-Quark-Quark Interaction	135
A.2. Neutralino-Neutralino-Higgs Interaction	135
A.3. Neutralino-Squark-Quark Interaction	136
 B. RelExt - Overview on the Mathematica Code and Direct Detection Class	 137
B.1. Mathematica Code	137
B.2. Direct Detection Class	141
 C. Benchmark Points used in the Analysis of Part III.	 143

Acknowledgements (Danksagungen)	149
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References	151
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CHAPTER 1

Introduction

The success story the Standard Model (SM) of particle physics has been underlined by the discovery of the Higgs boson in 2012 by the ATLAS [1] and CMS [2] collaborations at the Large Hadron Collider (LHC). However, even though the SM is able to explain many phenomena, there are questions that still remain unanswered, which indicates the existence of physics beyond the SM (BSM).

One of these open questions is the underlying nature of dark matter in the universe. The Standard Model of Cosmology is able to describe the evolution of the universe, while only being dependent on some parameters, which can be obtained by the measurement of the Cosmic Microwave Background [3]. From this measurement, we observe that $\sim 5\%$ of the energy budget of the universe is baryonic in nature, while $\sim 27\%$ consists of dark matter. It is assumed, that dark matter is electrically neutral, cold, i.e. moving at non-relativistic velocities, and collisionless, and has a lifetime longer than the age of the universe. Therefore dark matter solely interacts through the gravitational force and couples weakly to SM particles. The SM cannot provide a suitable dark matter candidate, thus we have to investigate BSM frameworks.

A promising type of candidates for dark matter are Weakly-Interacting-Massive Particles (WIMPs). The so-called WIMP-paradigm states that the experimentally measured dark matter relic abundance, which reads [3]

$$\Omega_c h^2 = 0.1200 \pm 0.0012 , \quad (1.1)$$

can be obtained with a dark matter particle with a mass and couplings to SM particles of the order of the electroweak scale. Extensions of the SM scalar sector can provide such WIMPs. In these Higgs portal models, the dark matter candidate communicates with the SM via a Higgs mediator. These models have two advantages. The first advantage is that extending the scalar sector of the SM provides us with a rich phenomenology which can be probed not only at the LHC, but also in future collider experiments. The second advantage is that the Higgs portal models can be probed in different and complimentary experiments in order to discover a possible dark matter signature. In direct detection experiments, one can use the Higgs boson as a mediator in dark matter-nucleus scattering [4]. At the time of writing this thesis, no signal in direct detection experiments has been measured. Nonetheless, these null results provide exclusion limits that constrain the parameter space of a given model.

Calculating the dark matter relic abundance can become tedious when dealing with models that include not one but multiple dark sector particles. To circumvent this issue, we have developed a tool that computes the relic density for an arbitrary dark matter model with a single dark matter candidate stabilized by a discrete symmetry. Additionally, we implemented algorithms to explore the parameter space in which the dark matter relic abundance agrees with the experimental measurement. In the literature, the dark matter relic density is, in most models, calculated only with leading-order diagrams. However, as experimental precision improves, theoretical predictions must also become more precise. Therefore, we will investigate in this thesis the impact of next-to-leading order electroweak and quantum chromodynamics (QCD) corrections on the dark matter relic abundance.

This thesis consists of five main parts. In Part I, we will first give an short overview of the SM (Sec. 2.1) and proceed with establishing the different BSM frameworks, which are the Complex Singlet Extension of the Standard Model (CxSM) (Sec. 2.2), the complex Two-Higgs Doublet Model (C2HDM) (Sec. 2.3) and the Next-to-Minimal Supersymmetric Standard Model (Sec. 2.4). Afterwards, we will provide a short introduction into the Standard Model of Cosmology in Ch. 3, and thereby develop the mathematical framework to calculate the dark matter relic abundance in Sec. 3.5 and the direct detection cross section in Sec. 3.6.

To give precise theoretical predictions, we need to understand the impact of experimental constraints on the parameter space in a given BSM theory. Therefore in Part II, we will investigate the interplay between collider constraints and the constraints of the electric dipole moment on the parameter space, by quantifying the allowed size of charge-parity (CP) violation in the fermionic couplings to the SM-like Higgs boson. We will first provide the expressions in order to calculate the electric dipole moment in Sec. 4.1. Afterwards, we will present the applied theoretical and experimental constraints and also the scan ranges of our input parameters in Ch. 5. In order to obtain our results, we will use two different approaches. In the first strategy, we will use a guided scan, while in the second strategy we will use machine learning algorithms in order to explore the parameter space. The results for the former case will be presented in Ch. 6. In Ch. 7, we will give a short overview on the used machine learning algorithm, which is succeeded by results using this technique. Finally, Ch. 8 will conclude this part.

In Part III, we will consider the Next-to-Minimal Supersymmetric Standard Model (NMSSM), where we developed the tool **NMSSMScanner**. As a proof-of-concept of our new tool, we maximize the cross section values for the production of a Higgs boson X , which subsequently decays into a pair consisting of a SM-like H plus non-SM-like Higgs boson Y , $X \rightarrow HY$ using a Markov-Chain-Monte-Carlo algorithm. Furthermore, the NMSSM provides a possible dark matter candidate, which is the lightest supersymmetric particle. Therefore we provide in Sec. 9.1, the framework how to calculate the dark matter relic abundance in the NMSSM. Furthermore, in Sec 9.2 we provide also an overview on how the direct detection cross section is obtained in the NMSSM. In Ch. 10, we present our dark matter tool RelExt, which is able to compute the dark matter relic abundance, assuming the freeze-out mechanism, for an arbitrary dark matter model where the dark matter particle is stabilized by a discrete symmetry. We furthermore extend the code by implementing the relic density and direct detection calculation for the NMSSM. In Ch. 11, we will present an overview of the tool **NMSSMScanner**, the additional observables tested and the computer codes used in the analysis. The results of our analysis will be presented in Ch. 12. Finally, in Ch. 13 will conclude this part.

In Part IV, we will investigate the impact of higher-order corrections on the dark matter relic density in the framework of the CxSM. We will first present how to obtain the dark matter relic density at next-to-leading order in Sec. 14.1. Here, ultraviolet and infrared divergences can arise. We will present in Ch. 15 how we treat these and show how to obtain ultraviolet- and infrared-finite annihilation cross sections. In Ch. 16, we present all relevant theoretical

and experimental constraints and provide the scan ranges of our parameter sample. In Ch. 17, we will present the results of our analysis. Finally, we will conclude this part with a summary and outlook in Ch. 18. Part V is the final part and consists of a summary and conclusion of this thesis.

Part I.

Theoretical Overview

Theories Beyond the Standard Model

As mentioned in the introduction, the SM has many unanswered questions, such as the hierarchy problem or the nature of dark matter. To address these problems, BSM theories are needed. In what follows, we first provide a brief overview of the SM. This is followed by the introduction of the BSM theories investigated in this thesis. Further, we will provide the necessary notation and conventions used throughout this thesis. For further information on the various models, references will be provided.

2.1. Standard Model of Particle Physics

The SM is a quantum field theory [5] that describes the fundamental particles and their interactions. Unifying the strong, weak, and electromagnetic forces into a single theory describes these interactions in terms of local gauge groups. The Lagrangian of the SM is invariant under local symmetry transformations of the gauge groups

$$SU(3)_C \times SU(2)_L \times U(1)_Y \quad . \quad (2.1)$$

The physics of quantum chromodynamics is encoded in the $SU(3)_C$ symmetry group, with the conserved quantum number color (C); the gauge fields that induce the strong interaction are the eight gluons G_μ^a ($a \in [1, \dots, 8]$). In contrast, the electroweak interaction unifies the weak and electromagnetic interactions and is described by the Glashow-Weinberg-Salam theory [6–8], whose underlying symmetry group is $SU(2)_L \times U(1)_Y$; the associated gauge fields for $SU(2)_L$ are W_μ^i ($i \in [1, 2, 3]$), while the gauge boson of $U(1)_Y$ is B_μ . To ensure local gauge invariance of the SM Lagrangian, the covariant derivative

$$\partial_\mu \rightarrow D_\mu = \partial_\mu - ig_s T^a G_\mu^a - ig_2 \frac{\sigma^i}{2} W_\mu^i - ig_1 Y B_\mu \quad (2.2)$$

is introduced. Here, g_s , g_2 , and g_1 denote the gauge coupling constants associated with the symmetry groups $SU(3)_C$, $SU(2)_L$, and $U(1)_Y$, respectively. The matrices T^a ($a \in [1, \dots, 8]$) are the generators of $SU(3)_C$. The generators of the weak isospin group $SU(2)_L$ are $\frac{\sigma_i}{2}$ ($i \in [1, 2, 3]$), where σ_i are the Pauli matrices. The hypercharge Y acts as the generator of the abelian $U(1)_Y$ group. This covariant derivative ensures that all fields in the theory

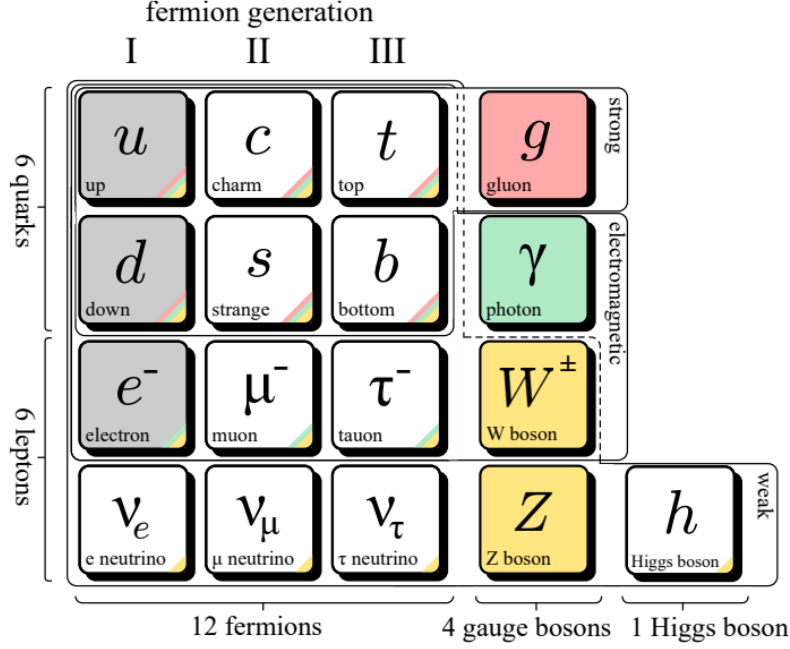


Figure 2.1.: Particle content of the SM. The fermionic particles, namely the quarks and leptons, have three generations. The gauge bosons mediate the three fundamental forces: the strong, weak, and electromagnetic. The Higgs boson is needed to give mass to the massive particles in the SM. The color markings on the various particle boxes indicate the forces they experience. The yellow indicates the weak interaction, green denotes the electromagnetic interaction, and red denotes the strong interaction. The responsible gauge boson, which mediates the corresponding force, is denoted by the color of the box. Taken from Ref. [9].

transform under local gauge transformations and preserve the internal symmetries of the SM. In Fig. 2.1, the particle content of the SM is depicted. It consists of spin-1/2 particles called fermions, spin-1 particles called gauge bosons, and a spin-0 particle called the Higgs boson. In the SM, all elementary particles, with the exception of neutrinos, gluons, and photons, acquire a mass. In the following sections, we discuss the mechanism responsible for mass generation within the SM.

2.1.1. The Higgs Mechanism

It has been experimentally shown that the weakly interacting gauge bosons are massive. However, including a mass term for the gauge bosons would break gauge invariance. The Higgs mechanism offers a solution to this problem. It was developed in the 1960s by Higgs, Englert, and Brout [10–12]. In this approach, a complex scalar doublet Φ is introduced. This field is charged under $SU(2)_L \times U(1)_Y$ and is given by

$$\Phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}, \quad (2.3)$$

where ϕ^0 and ϕ^+ are complex fields. The subscripts denote the electric charge Q , which can be obtained from the Gell-Mann-Nishijima relation

$$Q = I_3 + Y, \quad (2.4)$$

	Y	I_3	Q
ϕ^+	$\frac{1}{2}$	$\frac{1}{2}$	1
ϕ^0	$\frac{1}{2}$	$-\frac{1}{2}$	0

Table 2.1.: Quantum numbers of the Higgs doublet.

where I_3 and Y represent the third component of the weak isospin and the hypercharge, respectively. The corresponding quantum numbers of the fields ϕ^+ and ϕ^0 are given in Tab 2.1.

The Higgs Lagrangian $\mathcal{L}_\Phi$ is given by

$$\mathcal{L}_\Phi = (D^\mu \Phi)^\dagger (D_\mu \Phi) + \mu^2 \Phi^\dagger \Phi - \lambda (\Phi^\dagger \Phi)^2 \quad \text{with } \lambda, \mu^2 > 0. \quad (2.5)$$

The field Φ develops a non-vanishing vacuum-expectation value (VEV) in the ground state, which is given by

$$\langle 0 | \Phi | 0 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}. \quad (2.6)$$

It minimizes the potential term of Eq. (2.5). Using the minimization condition, one obtains the following relation

$$\left. \frac{dV}{d\Phi} \right|_{\Phi_0=v} = 0 \Rightarrow v = \sqrt{\frac{\mu^2}{2\lambda}}. \quad (2.7)$$

The VEV breaks the $SU(2)_L \times U(1)_Y$ symmetry spontaneously down to the electromagnetic $U(1)_{\text{em}}$, where the generator of this symmetry is given by the electric charge. The massless photon A_μ is the gauge boson of the $U(1)_{\text{em}}$ and is also the mediator of the electromagnetic force. The Goldstone-Theorem [13] states that for each broken degree of freedom, one obtains a Goldstone boson. In the case of the SM, we obtain three pseudo-Goldstone bosons and a massive scalar Higgs boson h . By choosing the unitary gauge, the Goldstone bosons are absorbed in the mass eigenstates of the electroweak gauge bosons $W^\pm$ and Z . After expansion around the minimum and the choice of the unitary gauge, the Higgs doublet reads as [14]

$$\Phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h \end{pmatrix} \quad (2.8)$$

We obtain the following mass term after inserting Eq. (2.8) into the kinetic term of Eq. (2.5)

$$\mathcal{L}_m = \frac{v^2}{8} \begin{pmatrix} W_\mu^1 \\ W_\mu^2 \\ W_\mu^3 \\ B_\mu \end{pmatrix}^T \begin{pmatrix} g_2^2 & 0 & 0 & 0 \\ 0 & g_2^2 & 0 & 0 \\ 0 & 0 & g_2^2 & -g_2 g_1 \\ 0 & 0 & -g_2 g_1 & g_1^2 \end{pmatrix} \begin{pmatrix} W_\mu^1 \\ W_\mu^2 \\ W_\mu^3 \\ B_\mu \end{pmatrix}, \quad (2.9)$$

where the mass eigenstates of the gauge bosons can be extracted as

$$W_\mu^\pm = \frac{1}{\sqrt{2}}(W_\mu^1 \mp iW_\mu^2) \quad , \quad (2.10)$$

$$Z_\mu = \frac{1}{\sqrt{g_2^2 + g_1^2}}(g_2 W_\mu^3 - g_1 B_\mu) \quad , \quad (2.11)$$

$$A_\mu = \frac{1}{\sqrt{g_2^2 + g_1^2}}(g_1 W_\mu^3 + g_2 B_\mu) \quad . \quad (2.12)$$

The corresponding mass eigenvalues are given by

$$m_W^2 = \frac{g_2^2 v^2}{4} \quad , \quad (2.13)$$

$$m_Z^2 = \frac{(g_1^2 + g_2^2)v^2}{4} \quad , \quad (2.14)$$

$$m_A^2 = 0 \quad . \quad (2.15)$$

The VEV v is then given by

$$v = 2 \frac{m_W}{g_2} \approx 246 \text{ GeV} \quad . \quad (2.16)$$

This value sets the scale for electroweak symmetry breaking.

The mass of the Higgs boson h can be obtained by inserting Eq. (2.8) into the potential term given in Eq. (2.5). The mass m_h then reads

$$m_h^2 = 4\lambda v^2 \quad . \quad (2.17)$$

The parameter λ is a free parameter in the SM, which means that the Higgs boson mass was unknown until 2012. The discovery of the Higgs boson by the ATLAS and CMS collaborations of the LHC [15,16] completed the SM, where the measured Higgs boson mass is given by [17]

$$m_h = (125.09 \pm 0.21 \pm 0.11) \text{ GeV} \quad . \quad (2.18)$$

2.1.2. Yukawa Sector

Adding a mass term for the fermions naively would lead to a violation of the chiral symmetry of the Lagrangian. However, this problem is cured by the Yukawa interaction of the fermions with the Higgs boson. In order to discuss the Higgs-fermion interaction, we will discuss the Higgs-quark interaction, which then be generalized for the leptonic case. Here, we will follow the description given in Ref. [5].

As there are three generations of quarks, we can arrange the quarks in three left-handed doublets and six right-handed singlets, which then reads

$$Q_L^i = \begin{pmatrix} u^i \\ d^i \end{pmatrix}_L = \left(\begin{pmatrix} u \\ d \end{pmatrix}_L, \begin{pmatrix} c \\ s \end{pmatrix}_L, \begin{pmatrix} t \\ b \end{pmatrix}_L \right) \quad , \quad (2.19)$$

and

$$u_R^i = (u_R, c_R, t_R), \quad d_R^i = (d_R, s_R, b_R) \quad . \quad (2.20)$$

In general, Higgs couplings will mix all the various quark flavours, unless we introduce a new discrete symmetry which would forbid such interactions. If we do not introduce such a symmetry the most general renormalizable gauge-invariant Higgs-quark interaction Lagrangian $\mathcal{L}_m$ reads

$$\mathcal{L}_m = -\lambda_d^{ij} \bar{Q}_L \Phi d_R - \lambda_u^{ij} \epsilon^{ab} \bar{Q}_{La} \Phi_b^\dagger u_R^\dagger + h.c. \quad , \quad (2.21)$$

where ϵ is given by

$$\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (2.22)$$

Further, λ_u^{ij} and λ_d^{ij} are general complex-valued matrices. Equation (2.21) would be invariant under charge (C) and parity (P) transformation, if the matrices λ^{ij} were real. However, there is no principle, which requires this to be true. Therefore, one could assume that the Higgs-quark interaction is violating all discrete and flavour symmetries. However, this is not the case as we can use chiral transformations to rewrite Eq. (2.21) in a more simplified form. In order to find the correct transformation, we square the Hermitian matrices Λ_i , which are given by the square of λ_i ($k \in [u, d]$). Further, we introduce unitary matrices U_i and W_i ($i \in [u, d]$), which are defined by

$$\lambda_i \lambda_i^\dagger = U_i D_i^2 U_i^\dagger, \quad \lambda_i^\dagger \lambda_i = W_i D_i^2 W_i^\dagger, \quad (2.23)$$

where D_i^2 is a diagonal matrix with positive eigenvalues. Therefore, the matrices λ_i are given by

$$\lambda_i = U_i D_i W_i^\dagger, \quad (2.24)$$

where the eigenvalues of the diagonal matrix D_i are the positive square roots of the eigenvalues of Eq. (2.23). Next, we transform our variables so that it reads

$$u_R^i \rightarrow W_u^{ij} u_R^j, \quad d_R^i \rightarrow W_d^{ij} d_R^j. \quad (2.25)$$

Using this transformation, the unitary matrices W_i disappear in the Higgs-quark interaction Lagrangian.³ The analogous transformation for the left-handed quarks reads

$$u_L^i \rightarrow U_u^{ij} u_L^j, \quad d_L^i \rightarrow U_d^{ij} d_L^j. \quad (2.26)$$

Using this transformation, the unitary matrices vanish in the terms that involve the lower component of the scalar field Φ . After inserting Eq. (2.8) and performing all mentioned transformations on Eq. (2.21), we obtain the following form of the interaction Lagrangian

$$\mathcal{L}_m = -m_d^i \bar{d}_L^i d_R^i \left(1 + \frac{h}{v}\right) - m_u^i \bar{u}_L^i u_R^i \left(1 + \frac{h}{v}\right) + h.c. . \quad (2.27)$$

Here, m_k^i ($i \in [1, 2, 3]$), ($k \in [u, d]$) denote the masses of the up- and down-type quark of the i -th generation. The mass relation is given by

$$m_k^i = D_k^{ii} \frac{v}{\sqrt{2}} \equiv y_k^i \frac{v}{\sqrt{2}}, \quad (2.28)$$

where we defined the eigenvalues of the diagonal matrices D_k^{ii} as the Yukawa couplings y_k^i . One can now perform the analogous steps for leptons, but we will not discuss them here. We will only present the resulting mass term for the leptons, which is given by

$$m_l = y_l \frac{v}{\sqrt{2}}, \quad (2.29)$$

where y_l denotes the Yukawa coupling between the lepton l ($l \in [e, \mu, \tau]$) to the Higgs boson.

³Actually, it disappears completely from the theory, as this transformation also leaves the kinetic terms of the right-handed quarks invariant. For a more detailed discussion, we refer to Ref. [5]

2.2. Complex Singlet Extension of the Standard Model

One of the simplest extensions of the SM is the CxSM [18–25]. In this model, the scalar sector of the SM is extended by an additional complex singlet $\mathbb{S}$. This singlet has zero isospin and hypercharge. After electroweak symmetry breaking, the fields can be expressed as

$$\Phi = \begin{pmatrix} G^+ \\ \frac{1}{\sqrt{2}}(v + H + iG^0) \end{pmatrix}, \quad \mathbb{S} = \frac{1}{\sqrt{2}}(v_s + S + i(v_A + A)) \quad . \quad (2.30)$$

Here, H , S , and A are real scalar fields. G^+ and G^0 are the charged and neutral Goldstone bosons, respectively. The VEVs of the fields H , S , and A are denoted as v , v_s , and v_A . A global $U(1)$ symmetry is applied to the singlet, which is softly broken. This results in the following renormalizable potential,

$$V_{\text{CxSM}} = \frac{m^2}{2}\Phi^\dagger\Phi + \frac{\lambda}{4}(\Phi^\dagger\Phi)^2 + \frac{\delta_2}{2}\Phi^\dagger\Phi|\mathbb{S}|^2 + \frac{b_2}{2}|\mathbb{S}|^2 + \frac{d_2}{4}|\mathbb{S}|^4 + \left(\frac{b_1}{4}\mathbb{S}^2 + a_1\mathbb{S} + c.c.\right) . \quad (2.31)$$

To obtain a stable dark matter candidate, two additional $\mathbb{Z}_2$ symmetries, $\mathbb{Z}_2^S$ and $\mathbb{Z}_2^A$, are enforced on the Lagrangian, such that it stays invariant under these transformations. The fields transform under this symmetry as follows

$$\mathbb{Z}_2^A : A \rightarrow -A, \quad \mathbb{Z}_2^S : S \rightarrow -S \quad . \quad (2.32)$$

Applying these symmetries, we obtain the following potential

$$V_{\text{CxSM}} = \frac{m^2}{2}\Phi^\dagger\Phi + \frac{\lambda}{4}(\Phi^\dagger\Phi)^2 + \frac{\delta_2}{2}\Phi^\dagger\Phi|\mathbb{S}|^2 + \frac{b_2}{2}|\mathbb{S}|^2 + \frac{d_2}{4}|\mathbb{S}|^4 + \left(\frac{b_1}{4}\mathbb{S}^2 + c.c.\right) . \quad (2.33)$$

Here, all m^2 , λ , δ_2 , b_2 , d_2 and b_1 are real parameters. Note that due to the two $\mathbb{Z}_2$ symmetries, the parameter b_1 is real and a_1 is set to zero compared to Eq. (2.31). Inserting Eq. (2.30) into this potential shows that H and S mix. This mixing can be parametrized by the relation

$$\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = R_\alpha \begin{pmatrix} H \\ S \end{pmatrix} \quad , \quad (2.34)$$

Here h_i ($i \in [1, 2]$) are the mass eigenstates, where by definition $m_{h_1} \leq m_{h_2}$. The rotation matrix R_α is given by

$$R_\alpha = \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{pmatrix} . \quad (2.35)$$

We can then define the mass matrix D_{hh}^2 for the mass eigenstates as

$$\text{diag}(m_{h_1}^2, m_{h_2}^2) \equiv D_{hh}^2 = R_\alpha \mathcal{M} R_\alpha^T \quad , \quad (2.36)$$

where $\mathcal{M}$ is the mass matrix for the gauge eigenstates. This matrix is given by

$$\mathcal{M} = \begin{pmatrix} \frac{v^2\lambda}{2} & \frac{\delta_2 v v_s}{2} \\ \frac{\delta_2 v v_s}{2} & \frac{d_2 v_s^2}{2} \end{pmatrix} + \begin{pmatrix} \frac{T_1}{v} & 0 \\ 0 & \frac{T_2}{v_s} \end{pmatrix} . \quad (2.37)$$

Here we used the tadpole parameters T_1 and T_2 , which are defined by

$$\frac{\partial V}{\partial v} \equiv T_1 \Rightarrow \frac{T_1}{v} = \frac{m^2}{2} + \frac{\delta_2 v_S^2}{4} + \frac{v^2 \lambda}{4} , \quad (2.38)$$

$$\frac{\partial V}{\partial v_S} \equiv T_2 \Rightarrow \frac{T_2}{v_S} = \frac{b_1 + b_2}{2} + \frac{\delta_2 v^2}{4} + \frac{v_S^2 d_2}{4} . \quad (2.39)$$

At tree-level $T_1 = T_2 = 0$, however, we keep these explicit as they require renormalization and therefore receive higher-order corrections. We will return to this in Part IV of this thesis. As the mass eigenstates are mixed states of H and S , the fields h_i ($i \in [1, 2]$) couple to SM particles. The couplings of h_i to two SM particles are given by

$$g_{h_i S M S M} = g_{H S M S M} k_i , \quad (2.40)$$

where the k_i are given by

$$k_i = \begin{cases} \cos(\alpha) & \text{for } i = 1 \\ -\sin(\alpha) & \text{for } i = 2 \end{cases} . \quad (2.41)$$

$$(2.42)$$

The mass m_A of the dark matter particle A is given by

$$m_A^2 = \frac{b_2 - b_1}{2} + \frac{\delta_2 v^2}{4} + \frac{v_S^2 d_2}{4} = -b_1 + \frac{T_2}{v_s} . \quad (2.43)$$

Now, it is possible to replace the six free parameters of the potential. These parameters are

$$m, \quad \lambda, \quad \delta_2, \quad b_2, \quad d_2, \quad b_1 , \quad (2.44)$$

They can be replaced by the following input parameters

$$v, \quad v_s, \quad m_{h_1}, \quad m_{h_2}, \quad m_A, \quad \alpha \quad (2.45)$$

2.3. The Complex Two-Higgs-Doublet-Model

In the framework of the Complex Two-Higgs-Doublet model (C2HDM) [26–34], the SM is extended by an additional complex scalar doublet. Furthermore, a softly broken $\mathbb{Z}_2$ symmetry, which is given by

$$\Phi_1 \rightarrow \Phi_1, \quad \Phi_2 \rightarrow -\Phi_2 , \quad (2.46)$$

is imposed. Here, Φ_1 and Φ_2 are the scalar doublets of the model. The potential reads

$$\begin{aligned} V_{\text{C2HDM}} = & m_{11}^2 |\Phi_1|^2 + m_{22}^2 |\Phi_2|^2 - (m_{12}^2 \Phi_1^\dagger \Phi_2 + h.c.) + \frac{\lambda_1}{2} (\Phi_2^\dagger \Phi_2)^2 + \frac{\lambda_2}{2} (\Phi_2^\dagger \Phi_2)^2 \\ & + \lambda_3 (\Phi_1^\dagger \Phi_1) (\Phi_2^\dagger \Phi_2) + \lambda_4 (\Phi_1^\dagger \Phi_2) (\Phi_2^\dagger \Phi_1) + \left[\frac{\lambda_5}{2} (\Phi_1^\dagger \Phi_2)^2 + h.c. \right] . \end{aligned} \quad (2.47)$$

The parameters λ_i ($i \in [1, 2, 3, 4]$) and the mass parameters m_{11}^2 and m_{22}^2 are real, while λ_5 and m_{12}^2 are complex parameters. The doublets can be written in terms of the complex charged fields ϕ_i^+ , the real neutral fields ρ_i and η_i and the vacuum expectation values v_i ($i \in [1, 2]$). The doublets are then given by

$$\Phi_1 = \begin{pmatrix} \phi_1^+ \\ \frac{1}{\sqrt{2}}(v_1 + \rho_1 + i\eta_1) \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} \phi_2^+ \\ \frac{1}{\sqrt{2}}(v_2 + \rho_2 + i\eta_2) \end{pmatrix} . \quad (2.48)$$

From the minimization conditions, we obtain three different equations

$$m_{11}^2 v_1 + \frac{\lambda_1}{2} v_1^3 + \frac{\lambda_{345}}{2} v_1 v_2^2 = \text{Re}(m_{12}^2) v_2 , \quad (2.49)$$

$$m_{22}^2 v_1 + \frac{\lambda_2}{2} v_2^3 + \frac{\lambda_{345}}{2} v_1^2 v_2 = \text{Re}(m_{12}^2) v_1 , \quad (2.50)$$

$$2\text{Im}(m_{12}^2) = v_1 v_2 \text{Im}(\lambda_5) . \quad (2.51)$$

Here we introduced the short-hand notation λ_{345} , which is given by

$$\lambda_{345} = \lambda_3 + \lambda_4 + \lambda_5 . \quad (2.52)$$

The Eqs. (2.49), (2.50) and (2.51) ensure that one CP-violating phase is obtained if $v_i \neq 0$ ($i \in [1, 2]$) and $\text{Im}(\lambda_5^*(m_{12}^2)^2) \neq 0$ [26–28]. In order to diagonalize the mass matrix, we first need to rotate into the Higgs basis [35–38]

$$\begin{pmatrix} \mathcal{H}_1 \\ \mathcal{H}_2 \end{pmatrix} = R_H^T \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = \begin{pmatrix} \cos \beta & \sin \beta \\ -\sin \beta & \cos \beta \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} , \quad (2.53)$$

where the angle β is given by the following relation

$$\tan \beta = \frac{v_2}{v_1} . \quad (2.54)$$

The doublets in this basis are then given by

$$\mathcal{H}_1 = \begin{pmatrix} G^+ \\ \frac{1}{\sqrt{2}}(v + H^0 + iG^0) \end{pmatrix}, \quad \mathcal{H}_2 = \begin{pmatrix} \phi_2^+ \\ \frac{1}{\sqrt{2}}(R_2 + iI_2) \end{pmatrix} , \quad (2.55)$$

where H^0 , R_2 and I_2 denote real fields. If we identify $\rho_3 \equiv I_2$, the mass eigenstates h_1, h_2 and h_3 are given by

$$\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = R \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix} = T^T \begin{pmatrix} H^0 \\ R_2 \\ I_2 \end{pmatrix} . \quad (2.56)$$

The orthogonal matrix R reads [39, 40]

$$R = \begin{pmatrix} c_1 c_2 & s_1 c_2 & s_2 \\ -(c_1 s_2 s_3 + s_1 c_3) & c_1 c_3 - s_1 s_2 s_3 & c_2 s_3 \\ -c_1 s_2 c_3 + s_1 s_3 & -(c_1 s_3 + s_1 s_2 c_3) & c_2 c_3 \end{pmatrix} , \quad (2.57)$$

where $s_i \equiv \sin \alpha_i$, $c_i \equiv \cos \alpha_i$ ($i \in [1, 2, 3]$). The Matrix T^T is defined as

$$T^T = R \begin{pmatrix} c_\beta & -s_\beta & 0 \\ s_\beta & c_\beta & 0 \\ 0 & 0 & 1 \end{pmatrix} \equiv \begin{pmatrix} q_{11} & \text{Re}(q_{12}) & \text{Im}(q_{12}) \\ q_{21} & \text{Re}(q_{22}) & \text{Im}(q_{22}) \\ q_{31} & \text{Re}(q_{32}) & \text{Im}(q_{32}) \end{pmatrix} , \quad (2.58)$$

Note, that we adopted the notation for the matrix elements in the last equality from Ref. [41], such that we can use it in the calculation of the electron electric dipole moment in Part II of this thesis. The mass matrix of the neutral scalars is given by

$$(\mathcal{M}^2)_{ij} = \left\langle \frac{\partial^2 V_{\text{C2HDM}}}{\partial \rho_i \partial \rho_j} \right\rangle, \quad (2.59)$$

where the notation $\langle \dots \rangle$ denotes, that the scalar fields ρ_i and ρ_j are evaluated at the VEVs of the fields. This mass matrix is then diagonalized as

$$\text{diag}(m_1, m_2, m_3) = R \mathcal{M}^2 R^T. \quad (2.60)$$

Here, the masses of the neutral Higgs bosons are ordered such that $m_1 \leq m_2 \leq m_3$. Further, the model contains, in addition to the three neutral particles, two charged scalars, $H^\pm$. The set of independent input parameters is then given by

$$\tan \beta, \quad m_{H^\pm}, \quad \alpha_1, \quad \alpha_2, \quad \alpha_3, \quad m_{h_1}, \quad m_{h_2}, \quad \text{Re}(m_{12}^2). \quad (2.61)$$

Using these input parameters, the mass of the heaviest scalar m_3 is a derived quantity, such that it reads

$$m_3 = \frac{m_1^2 R_{13}(R_{12} \tan \beta - R_{11}) + m_2^2 R_{23}(R_{22} \tan \beta - R_{12})}{R_{33}(R_{31} - R_{32} \tan \beta)} \quad (2.62)$$

The couplings of the neutral scalar particle h_i to a gauge boson V ($V \in [W^\pm, Z]$) is given by

$$g_{h_i V V} = c(h_i V V) g_{h_{SM} V V}, \quad (2.63)$$

where $g_{\mu\nu}$ is the metric in Minkowski space, h_{SM} denotes the SM-like Higgs boson and $g_{h_{SM} V V}$ denotes the coupling of the SM-like Higgs boson to a massive gauge boson pair VV , which is given by

$$g_{h_{SM} V V} = \begin{cases} \frac{em_W}{\sin \theta_W}, & \text{for } V = W, \\ \frac{em_Z}{\sin \theta_W \cos \theta_W}, & \text{for } V = Z. \end{cases} \quad (2.64)$$

where e is the electric charge.

Yukawa Sector of the C2HDM

As a result of the extension of the scalar sector by an additional Higgs doublet, the Yukawa sector can, in general, develop flavor-changing neutral currents (FCNC) at tree level. In order to avoid this, we ensure that each right-handed fermion couples to only one Higgs doublet, by extending the $\mathbb{Z}_2$ symmetry to the fermion fields, such that it reads [42, 43]

$$\bar{Q}_L \rightarrow (-1)^a \bar{Q}_L, \quad d_R \rightarrow (-1)^b, \quad u_R \rightarrow (-1)^c \bar{u}, \quad \bar{L}_L \rightarrow (-1)^d \bar{L}_L, \quad l_R \rightarrow (-1)^e l_R. \quad (2.65)$$

Here, a, b, c, d, e are coefficients which can take the values 0 and 1. As we have four different combinations for the power of the exponents, we obtain four different types of C2HDM, which are the Type I, Type II, Lepton-specific (LS), and Flipped. In Tab. 2.2, we list the values of the exponents and the Higgs doublet which the right-handed fermion fields couple to in each type of the C2HDM. After electroweak symmetry breaking and diagonalizing the fields, we can write the interaction between the neutral scalars and fermions in the following Lagrangian $\mathcal{L}_{\text{Yukawa}}^h$, which reads

$$\mathcal{L}_{\text{Yukawa}}^h = \sum_{i=1}^3 \frac{m_f}{v} h_i \bar{f} [c^e(h_i f f) + i c^o(h_i f f) \gamma_5] f, \quad (2.66)$$

Type of C2HDM	a	b	c	d	e	u_R	d_R	l_R
Type I	0	1	1	0	1	Φ_2	Φ_2	Φ_2
Type II	0	0	1	0	0	Φ_2	Φ_1	Φ_1
Lepton-Specific	0	1	1	0	0	Φ_2	Φ_2	Φ_1
Flipped	0	0	1	0	1	Φ_2	Φ_1	Φ_2

Table 2.2.: Values of the exponents a, b, c, d, e and the Higgs doublet to which the right-handed fermion fields u_R, d_R and l_R couple to for each type of the C2HDM. Taken from Ref. [44].

where m_f denotes the mass of the fermion f . Here, we introduced the CP-even coupling

$$c^e(h_i f \bar{f}) = q_{i1} - 2T_3^f c_f \text{Re}(q_{i2}) , \quad (2.67)$$

where T_3^f is the isospin and c_f is the coupling coefficients of the fermion f , respectively. The CP-odd couplings reads

$$c^o(h_i f \bar{f}) = c_f \text{Im}(q_{i2}) . \quad (2.68)$$

Further, the coupling coefficients for down-type quarks, c_d , and charged leptons, c_l , depend on the specific type of the C2HDM and are given by [41]

$$\text{Type I : } c_d = c_l = \cot \beta , \quad (2.69)$$

$$\text{Type II : } c_d = c_l = -\tan \beta , \quad (2.70)$$

$$\text{LS : } \begin{cases} c_d = \cot \beta \\ c_l = -\tan \beta \end{cases} , \quad (2.71)$$

$$\text{Flipped : } \begin{cases} c_d = -\tan \beta \\ c_l = \cot \beta \end{cases} , \quad (2.72)$$

while for the coupling modifier for up-type quarks, it is in all types of C2HDM given by

$$c_u = -\cot \beta . \quad (2.73)$$

2.4. Next-to-Minimal Supersymmetric Standard Model

In this section, we will briefly introduce the NMSSM. Here, we will follow the reviews [45, 46] and the works of [9, 47].

The NMSSM goes beyond the minimal supersymmetric extension of the SM, the MSSM. While in the MSSM the SM scalar sector is extended by an additional scalar doublet, the NMSSM adds an additional scalar singlet field. Further, each field is promoted to a superfield, which contains both SM (and the additional scalar doublet and singlet) degrees of freedom and the ones of their supersymmetric partner, the superpartner. These superpartners differ from the SM particles only in their spin quantum number by $1/2$. This leads to the following particle content

- The fermions of the SM, obtain spin-0 superpartners, the sfermions. Accordingly, the superpartners of quarks leptons are therefore called squarks and sleptons, respectively.

- Compared to the SM, the Higgs sector is extended by an additional Higgs doublet and scalar singlet. The respective superpartners of the Higgs fields are spin- $\frac{1}{2}$ fermions, which are called higgsinos.
- The gauge bosons, i.e. the gluon as well as the W - and B -bosons as the gauge eigenstates of the $SU(2)_L$ and $U(1)_Y$ symmetries, have fermionic superpartners, called gauginos. In particular, these are called gluino, wino, and bino.

In Tab. 2.3, we list the field content and their quantum numbers of the NMSSM, which is identical to the field content of the MSSM [48], except for the additional singlet superfield $\hat{S}$. Here, all chiral superfields are denoted with a hat, while the superpartners of the SM fields are indicated by a tilde.

This additional superfield $\hat{S}$ is not charged under the SM gauge group. The superpotential $\mathcal{W}_{\text{NMSSM}}$ of the NMSSM then reads

$$\mathcal{W}_{\text{NMSSM}} = \mathbf{Y}_u \hat{u}(\hat{Q}^T \epsilon \hat{H}_u) - \mathbf{Y}_e \hat{e}(\hat{L}^T \epsilon \hat{H}_d) - \mathbf{Y}_d \hat{d}(\hat{Q}^T \epsilon \hat{H}_d) + \lambda \hat{S}(\hat{H}_u^T \epsilon \hat{H}_d) + \frac{1}{3} \kappa \hat{S}^3 \quad . \quad (2.74)$$

Here, $\mathbf{Y}_i$ ($i \in [e, u, d]$) are 3×3 Yukawa matrices which, for simplicity, will be already assumed diagonal with the quark and lepton fields corresponding to their mass eigenstates, λ and κ are the couplings between the Higgs superfields $\hat{H}_i$ ($i \in [u, d]$) and the singlet superfield $\hat{S}$ and ϵ is given by

$$\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad . \quad (2.75)$$

Furthermore, a $\mathbb{Z}_3$ symmetry is imposed such that there are no dimensionful terms in the superpotential. Since the superpartners have the same masses as the corresponding SM particles and experimentally, no supersymmetric particle has been found to date, additional terms have to be introduced that give additional mass terms only to the scalar particles thus explicitly breaks supersymmetry (SUSY). In the absence of any knowledge about a specific supersymmetry-breaking mechanism, these mass terms and additional interaction terms with couplings of positive mass dimension, such that the Lagrangian stays renormalizable are parametrized in the soft SUSY-breaking Lagrangian, which is given by

$$\begin{aligned} \mathcal{L}_{\text{soft, NMSSM}} = & -m_{H_u}^2 |H_u|^2 - m_{H_d}^2 |H_d|^2 - m_{\tilde{Q}}^2 \tilde{Q}^\dagger \tilde{Q} - m_{\tilde{L}}^2 \tilde{L}^\dagger \tilde{L} \\ & - m_{\tilde{u}_R}^2 \tilde{u}_R^* \tilde{u}_R - m_{\tilde{d}_R}^2 \tilde{d}_R^* \tilde{d}_R - m_{\tilde{l}_R}^2 \tilde{l}_R^* \tilde{l}_R \\ & - (-\mathbf{T}_l H_d^T \epsilon \tilde{L} \tilde{l}_R^* - \mathbf{T}_d H_d^T \epsilon \tilde{Q} \tilde{d}_R^* + \mathbf{T}_u H_u^T \epsilon \tilde{Q} \tilde{u}_R^* \\ & + \frac{M_1}{2} \tilde{B} \tilde{B} + \frac{M_2}{2} \tilde{W} \tilde{W} + \frac{M_3}{2} \tilde{G} \tilde{G} + h.c.) \\ & - m_S^2 |S|^2 + (T_\lambda S H_d^T \epsilon H_u - \frac{1}{3} T_\kappa S^3 + h.c.) \quad . \end{aligned} \quad (2.76)$$

Here, M_i ($i \in [1, 2, 3]$) are the complex masses parameters for the gauginos, while m_i^2 ($i \in [\tilde{Q}, \tilde{L}, \tilde{u}_R, \tilde{d}_R, \tilde{l}_R]$) are the real squared mass parameters for the sfermions. In addition, m_i^2 ($i \in [H_u, H_d, S]$) represent the real squared mass parameters of the Higgs doublets and the singlet field. The complex trilinear couplings $\mathbf{T}_i$ ($i \in [e, u, d]$) and T_i ($i \in [\lambda, \kappa]$) are defined as

$$T_\alpha \equiv \alpha A_\alpha \quad (\alpha \in [\lambda, \kappa]) \quad , \quad (2.77a)$$

$$\mathbf{T}_i \equiv \mathbf{Y}_i \mathbf{A}_i \quad (i \in [e, u, d]) \quad , \quad (2.77b)$$

where A_i is a complex parameter. Note, that $\mathbf{T}_i$ and $\mathbf{A}_i$ are complex 3×3 matrices. The scalar potential of the NMSSM focussing only on the terms containing the Higgs doubles H_u , H_d and the singlet S , is given by

$$\begin{aligned} V_{\text{NMSSM}} = & |\lambda|^2 |S|^2 (H_u^\dagger H_u + H_d^\dagger H_d) + |\lambda(H_u^T \epsilon H_d) + \kappa S|^2 \\ & + \frac{1}{2} g_2^2 |H_u^\dagger H_d|^2 + \frac{1}{8} (g_1^2 + g_2^2) (H_u^\dagger H_u - H_d^\dagger H_d)^2 \\ & + m_{H_u}^2 H_u^\dagger H_u + m_{H_d}^2 H_d^\dagger H_d + m_S^2 |S|^2 \\ & + (\lambda A_\lambda (H_u^T \epsilon H_d) S + \frac{1}{3} \kappa A_\kappa S^3 + c.c.). \end{aligned} \quad (2.78)$$

After electroweak symmetry breaking, the scalar doublets H_d , H_u and the singlet field S obtain a VEV and can be parametrized by

$$\begin{aligned} H_d = & \begin{pmatrix} \frac{1}{\sqrt{2}}(v_d + h_d + ia_d) \\ H_d^- \end{pmatrix}, \quad H_u = e^{i\varphi_u} \begin{pmatrix} H_u^+ \\ \frac{1}{\sqrt{2}}(v_u + h_u + ia_u) \end{pmatrix}, \\ S = & \frac{1}{\sqrt{2}} e^{i\varphi_s} (v_s + h_s + ia_s). \end{aligned} \quad (2.79)$$

Here, φ_i ($i \in [u, s]$) denote the phases, v_j the VEVs, h_j and a_j ($j \in [u, d, s]$) the real and pseudoscalar field components. The charged field components are given by H_u^+ and H_d^- . The angle β between the VEV directions is defined as

$$\tan \beta = \frac{v_u}{v_d}. \quad (2.80)$$

The two doublet VEVs have to fulfill the following relation

$$v^2 = v_u^2 + v_d^2, \quad (2.81)$$

where v is the SM VEV. The parameter μ_{eff} , which couples the two Higgs doublet superfields, is generated dynamically through the singlet VEV, such it reads

$$\mu_{\text{eff}} = \frac{\lambda v_s e^{i\varphi_s}}{\sqrt{2}}. \quad (2.82)$$

From the tadpole condition

$$\left\langle \frac{\partial V_{\text{NMSSM}}}{\partial \phi_i} \right\rangle = 0, \quad (2.83)$$

where $\phi_i = h_u, h_d, h_s, a_u, a_d, a_s$, we obtain a set of equation, which allows us to rewrite the potential parameters in terms of the following chosen input parameters

$$\begin{aligned} & \tan \beta, \lambda, \mu_{\text{eff}}, \varphi_s, \kappa, M_{H^\pm}, \varphi_u, \mathbf{A}_u, \mathbf{A}_d, \mathbf{A}_l, M_1, M_2, M_3 \\ & m_{\tilde{Q}}, m_{\tilde{L}}, m_{\tilde{u}_R}, m_{\tilde{d}_R}, m_{\tilde{t}_r}. \end{aligned} \quad (2.84)$$

The additional input parameters are the SM parameters which are the masses of the Z and W boson, the masses of the SM fermions, the fine structure constant α_{em} , and the strong coupling constant α_s .

The mass eigenstates of the neutral Higgs particles h_i^0 ($i \in [1, 2, 3, 4, 5]$) are obtained by applying two rotations to the gauge eigenstates, which read

$$\begin{aligned} (h_d, h_u, h_s, a, a_s, G^0)^T &= \mathcal{R}^G (h_d, h_u, h_s, a_d, a_u, a_s)^T \\ (h_1^0, h_2^0, h_3^0, h_4^0, h_5^0, G^0)^T &= \mathcal{R} (h_d, h_u, h_s, a, a_s, G^0)^T. \end{aligned} \quad (2.85)$$

The first rotation is performed to single out the would-be Goldstone boson and the second one performs the rotation into the mass eigenstates. The matrix $\mathcal{R}^G$ reads

$$\mathcal{R}^G = \begin{pmatrix} 1_{3 \times 3} & 0 \\ 0 & \tilde{\mathcal{R}}^G \end{pmatrix}, \quad \tilde{\mathcal{R}}^G = \begin{pmatrix} s_\beta & c_\beta & 0 \\ 0 & 0 & 1 \\ c_\beta & -s_\beta & 0 \end{pmatrix}. \quad (2.86)$$

The diagonal matrix mass matrix⁴ is given by

$$\text{diag}(m_{h_1^0}^2, m_{h_2^0}^2, m_{h_3^0}^2, m_{h_4^0}^2, m_{h_5^0}^2, m_{G^0}^2) = \mathcal{R} \mathcal{M}_{hh} \mathcal{R}^T, \quad \mathcal{M}_{hh} = \mathcal{R}^G \mathcal{M}_{\phi\phi} (\mathcal{R}^G)^T, \quad (2.87)$$

where $\mathcal{M}_{\phi\phi}$ denotes the neutral Higgs mass matrix in the gauge eigenbasis. All masses of all are sorted in ascending order⁵. Note, that in the CP-conserving case, which is the framework in which we work in this thesis, the CP-even and CP-odd eigenstates do not mix. Therefore the neutral Higgs sector consists of three CP-even neutral states h_i^0 ($i \in [1, 2, 3]$) and the two CP-odd states A_j ($j \in [1, 2]$).

The charged scalar mass eigenstates are obtained by

$$\begin{pmatrix} G^- \\ H^- \end{pmatrix} = \mathcal{R}^{G^-} \begin{pmatrix} h_d^- \\ h_u^- \end{pmatrix}, \quad \text{diag}(m_{H^\pm}^2, m_{G^\pm}^2) = \mathcal{R}^{G^-} \mathcal{M}_{h^+h^-} (\mathcal{R}^{G^-})^T, \quad (2.88)$$

with

$$\mathcal{R}^{G^-} = \begin{pmatrix} -c_\beta & s_\beta \\ s_\beta & c_\beta \end{pmatrix}. \quad (2.89)$$

The neutral higgsinos $\tilde{H}_u^0, \tilde{H}_d^0, \tilde{S}$ and the gauginos $\tilde{B}$ and $\tilde{W}$ mix with a mixing matrix $\mathcal{N}$. The resulting mass eigenstates, the neutralinos, are denoted as $\tilde{\chi}_i^0$ ($i \in [1, 2, 3, 4, 5]$), and have the following diagonalized mass matrix which reads

$$\text{diag}(m_{\tilde{\chi}_1^0}, m_{\tilde{\chi}_2^0}, m_{\tilde{\chi}_3^0}, m_{\tilde{\chi}_4^0}, m_{\tilde{\chi}_5^0}) = \mathcal{N}^* \mathcal{M}_{\tilde{\chi}_0} \mathcal{N}^\dagger. \quad (2.90)$$

Here, $\mathcal{M}_{\tilde{\chi}_0}$ denotes the neutralino mass matrix in the gauge eigenbasis with the above higgsino and gaugino states. The neutralinos are Majorana fermions, and the lightest neutralino, which in many supersymmetric scenarios is also the lightest supersymmetric particle, is then considered a dark matter candidate. We will come back to this in Part III of this thesis. Similarly, the charged higgsinos $\tilde{H}_u^\pm, \tilde{H}_d^\pm$ mix with the charged gauginos $\tilde{W}$. Here, we obtain a mass matrix $\mathcal{M}_{\tilde{\chi}^\pm}$ which is diagonalized by two rotation matrices $\mathcal{V}$ and $\mathcal{U}$. The mass eigenstates resulting of this mixing are the charginos $\tilde{\chi}_i^\pm$ ($i \in [1, 2]$). Their masses are given by

$$\text{diag}(m_{\tilde{\chi}_1^\pm}, m_{\tilde{\chi}_2^\pm}) = \mathcal{U}^* \mathcal{M}_{\tilde{\chi}^\pm} \mathcal{V}^\dagger. \quad (2.91)$$

Lastly, the sfermions generally mix. Here, we obtain the mass matrix $\mathcal{M}_{\tilde{f}}$ with a rotation matrix $W^{\tilde{f}}$ for each type of sfermion $\tilde{f}$ ($f \in [e, \mu, \tau, u, c, t, d, s, b, \nu_e, \nu_\mu, \nu_\tau]$). The masses of the sfermions are then given by

$$\text{diag}(m_{\tilde{f}_1}, m_{\tilde{f}_2}) = W^{\tilde{f}} \mathcal{M}_{\tilde{f}} W^{\tilde{f}\dagger} \quad (2.92)$$

Here, we consider only mixing between the supersymmetric partners of the right- and left-handed fields and no flavor mixing. The presentation of the mass matrices is omitted, and we refer here to the literature [45, 48, 49].

This concludes the chapter, in which we introduced all relevant models used in this work.

⁴Note, that we work in the 't Hooft-Feynman gauge, which in turn means that the neutral and charged Goldstone bosons have the same masses as the Z and $W^\pm$ bosons, respectively.

⁵This is assumed to be true for all mass eigenstates in the following.

	Superfield	Spin-0	Spin- $\frac{1}{2}$	$SU_C(3) \times SU_L(2) \times U_Y(1)$
Higgs-Higgsino	$\hat{H}_u$	$H_u = (H_u^+, H_u^0)^T$	$\tilde{H}_u = (\tilde{H}_u^+, \tilde{H}_u^0)^T$	$\left(1, 2, \frac{1}{2}\right)$
	$\hat{H}_d$	$H_d = (H_d^0, H_d^-)^T$	$\tilde{H}_d = (\tilde{H}_d^0, \tilde{H}_d^-)^T$	$\left(1, 2, -\frac{1}{2}\right)$
	$\hat{S}$	S	$\tilde{S}$	$(1, 1, 0)$
Quark-Squark	$\hat{Q}$	$\tilde{Q} = (\tilde{u}_L, \tilde{d}_L)^T$	$Q = (u_L, d_L)^T$	$\left(3, 2, \frac{1}{6}\right)$
	$\hat{u}$	$\tilde{u}_R^*$	$u_R^\dagger$	$\left(\bar{3}, 1, -\frac{2}{3}\right)$
	$\hat{d}$	$\tilde{d}_R^*$	$d_R^\dagger$	$\left(\bar{3}, 1, \frac{1}{3}\right)$
Lepton-Slepton	$\hat{L}$	$\tilde{L} = (\tilde{\nu}, \tilde{l}_L)^T$	$L = (\nu, l_L)^T$	$\left(1, 2, -\frac{1}{2}\right)$
	$\hat{l}$	$\tilde{l}_R^*$	$l_R^\dagger$	$(1, 1, 1)$
		Spin-1	Spin- $\frac{1}{2}$	
B-Bino	$\hat{B}$	B	$\tilde{B}$	$(1, 1, 1)$
W-Wino	$\hat{W}$	W	$\tilde{W}$	$(1, 3, 0)$
gluon-gluino	$\hat{g}$	g	$\tilde{G}$	$(8, 1, 0)$

Table 2.3.: Field content and the corresponding quantum numbers of the NMSSM [45]. The subscripts R and L denote the right- and left-handed fermions. The subscripts of the scalar particle indicate to which fermions they are related to.

Brief Overview of the Standard Model of Cosmology

One of the most sought-after problems in modern physics is the existence of dark matter. Little is known about the nature and properties of dark matter. However, there is multiple evidence (cf. Refs. [3,50,51]). To compute and study dark matter observables, it is necessary to first establish the theoretical framework in which these quantities can be consistently defined and evaluated. This framework is the so-called Standard Model of Cosmology. Note that explaining it in its full complexity is beyond the scope of this thesis. We therefore refer to Refs. [52–54] for a more comprehensive overview. In this work, we will focus only on aspects relevant to understanding the thermal history of the universe and to calculating dark matter observables, in particular, the relic density. Here, we follow the description given in Ref. [53].

3.1. General Relativity

We start our description with Einstein's field equations (EFEs), which read

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi G T_{\mu\nu}. \quad (3.1)$$

Here, $G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R$ denotes the Einstein tensor, which represents the curvature of space-time, $R_{\mu\nu}$ is the Ricci tensor, R the Ricci scalar, G is the gravitational constant, $g_{\mu\nu}$ is the metric tensor and Λ is the cosmological constant. Further, $T_{\mu\nu}$ denotes the energy momentum tensor, which reads

$$T_{\mu\nu} = (\rho + p)u_\mu u_\nu + pg_{\mu\nu} + q_\mu u_\nu + u_\mu q_\nu + \pi_{\mu\nu}, \quad (3.2)$$

where u_μ is the velocity four-vector, ρ the energy density, p denotes the isotropic pressure, q_μ is the energy flux and $\pi_{\mu\nu}$ is the anisotropic pressure. Also, ρ , p , q_μ and $\pi_{\mu\nu}$ are dependent on space and time. In the Standard Model of Cosmology, it is assumed that the cosmic fluid behaves as a perfect fluid, i.e., $q_\mu = 0$ and $\pi_{\mu\nu} = 0$, corresponding to a large-scale homogeneous and isotropic description of the universe. The energy-momentum tensor then reduces to

$$T_{\mu\nu} = (\bar{p} + \bar{\rho})u_\mu u_\nu + \bar{p}g_{\mu\nu}. \quad (3.3)$$

Here, the bar over the quantities denotes the spatial average, so that they now depend only on time.⁶ Numerous solutions to the EFEs have been proposed. In this work, however, we focus on the homogeneous and isotropic Friedmann–Lemaître–Robertson–Walker (FLRW) solutions [55–58], which we discuss in the next section.

3.2. Friedmann-Lemaître-Robertson-Walker Metric and the Friedmann Equations

From the cosmological principle and the observation that the universe is, at large scales, isotropic, it can be assumed that spacetime is homogeneous and isotropic. The line element is then given by

$$ds = dt - a^2(t) \left(\frac{dr^2}{1 - kr^2} + r^2(d\theta^2 + \sin^2(\theta)d\phi^2) \right), \quad (3.4)$$

where r is the radial component, t is the time, the angular variables are denoted as θ and ϕ , $a(t)$ is the scale factor⁷, and $k = -1, 0, 1$ denotes the curvature constant. The value of k depends on whether the universe is open (-1), closed (1), or spatially flat (0). The Friedmann equations are obtained, after solving the EFEs for the metric given in Eq. (3.4) and the energy-momentum tensor given in Eq. (3.3). The first equation is obtained for the case $\mu = \nu = 0$ and reads

$$\frac{\dot{a}^2}{a^2} \equiv H^2(t) = \frac{8\pi G}{3}\rho + \frac{\Lambda}{3} - \frac{k}{a^2}. \quad (3.5)$$

Here, the dot over a quantity denotes its time derivative, and we have introduced the Hubble parameter $H(t)$. The Hubble constant H_0 is obtained by inserting the current time t_0 , so that it reads

$$H_0 = H(t_0). \quad (3.6)$$

The second Friedmann equation follows from combining the 00-component and the spatial ii -components of the EFEs and is given by

$$\frac{\ddot{a}}{a} = \frac{-4\pi G}{3}(\rho + 3p) + \frac{\Lambda}{3}. \quad (3.7)$$

The FLRW metric and the Friedmann equations describe a homogeneous and isotropic universe and its dynamics. With these, we can now study the energy budget of the universe, which we will describe in the following section.

3.3. Energy Budget of the Universe

The conservation laws in general relativity are given by the following condition

$$\nabla^\nu T_{\mu\nu} = 0, \quad (3.8)$$

where ∇^ν denotes the covariant derivative. From Eq. (3.8), we obtain the continuity equation

$$\dot{\rho} + 3H(\rho + p) = \dot{\rho} + 3H\rho(1 + w) = 0. \quad (3.9)$$

Here, we introduced the equation of state variable w , which is given by

$$p = w\rho. \quad (3.10)$$

⁶In the following, we will drop the bar, however, the quantities should still be understood only as a function of time.

⁷We will omit the explicit time dependence on the scale factor in the following.

Using Eq. (3.9), we can derive that in a matter-dominated epoch, i.e. $w = 0$, the energy density ρ_m is proportional to a^{-3} , for a radiation dominated epoch, i.e. $w = 1/3$, $\rho_r \propto a^{-4}$ and for the cosmological constant, i.e. $w = -1$, ρ_Λ is a constant. The energy density for dynamical dark energy with a cosmological parameter w_{de} , which is dependent on the cosmological model, is proportional to $a^{-3(1+w_{\text{de}})}$.

Next, we will introduce the critical density ρ_c of the universe as evaluated today to describe the energy budget of the universe as measured by observations. We assume that the universe is spatially flat ($k = 0$) and the cosmological constant equals zero. From the first Friedmann equation, we then obtain

$$\rho_c = \frac{3H_0^2}{8\pi G} . \quad (3.11)$$

Using the critical density ρ_c , we can rewrite the first Friedmann equation in terms of the density ratios Ω_i ($i \in [m, r, k, \text{de}]$) which are given by

$$\Omega_i = \frac{\rho_i}{\rho_c} , \quad (3.12)$$

and the Friedman equation is then given by

$$\frac{H^2}{H_0^2} = \Omega_m a^{-3} + \Omega_r a^{-4} + \Omega_k a^{-2} + \Omega_{\text{de}} a^{-3(1+w)} . \quad (3.13)$$

Note, that we used $\Omega_m = \Omega_b + \Omega_c$, where Ω_b denotes the baryon content and Ω_c denotes the dark matter content. Further, we introduced a curvature density $\Omega_k \equiv -k/H_0^2 < 0.01$ [3]. These cosmological parameters, which define the Standard Model of Cosmology, are measured by the PLANCK collaboration from the cosmic microwave background (CMB), which we will discuss in the next section.

3.4. Cosmic Microwave Background

For the probe the parameters of the Lambda Cold dark matter model (Λ CDM), which acts as the Standard Model of Cosmology, measurements of the CMB play an important role. Around 400,000 years after the Big Bang, the universe became transparent for light. This is because electrons and protons were able to form hydrogen atoms around this time. The decoupling point of photons from the universe is called the surface of last scattering [59]. Photons from this time period make up the CMB. As the universe is expanding, the temperature of the CMB decreases. The mean temperature of the CMB has been measured to be [3]

$$T_\gamma = (2.7255 \pm 0.006) \text{ K} . \quad (3.14)$$

The temperature of the CMB shows fluctuations $\frac{\delta T_\gamma}{T}$ of order 10^{-5} . These fluctuations can serve as a window into the beginning of the universe and its energy content. The fluctuations on the surface of last scattering are commonly parametrized by a spherical harmonic expansion, such that it reads

$$\frac{\delta T}{T_\gamma} = \sum_{l=0}^{\infty} \sum_{m=-l}^l a_{lm} Y_{lm}(\theta, \phi) , \quad (3.15)$$

where a_{lm} are expansion coefficients, θ and ϕ denote the angular variables, Y_{lm} are the spherical harmonics, l is the multipole moment, and m is the magnetic quantum number.

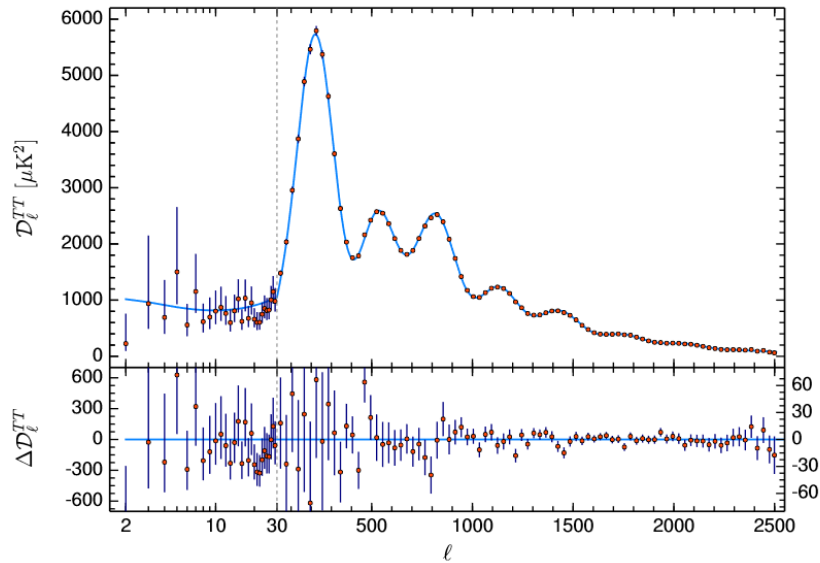


Figure 3.1.: Measured power spectrum over the dipole parameter l from the PLANCK experiment. Taken from [3].

In order to analyze the temperature anisotropies, it is useful to consider the variance of the temperature distribution, which is given by

$$\frac{1}{4\pi} \int d\Omega \left(\frac{\delta T}{T_\gamma} \right)^2 = \frac{1}{4\pi} \sum_{lm} |a_{lm}|^2 \quad . \quad (3.16)$$

Here, we used the fact that the spherical harmonics are orthonormal

$$\int Y_{lm}(\theta, \phi) Y_{l'm'}^* d\Omega = \delta_{ll'} \delta_{mm'} \quad . \quad (3.17)$$

As the surface of last scattering does not have a special direction in an isotropic universe, we can safely sum over m , as the expansion parameters a_{lm} do not depend on m . We can, therefore, define the power spectrum C_l , which is given the average of $|a_{lm}|^2$ over m as

$$C_l = \frac{1}{2l+1} \sum_{m=-l}^l |a_{lm}|^2 \quad . \quad (3.18)$$

Using Eq. (3.18), Eq. (3.16) then reads

$$\frac{1}{4\pi} \int d\Omega \left(\frac{\delta T}{T_\gamma} \right)^2 = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} C_l \quad . \quad (3.19)$$

In Fig. 3.1, the power spectrum measurement of the PLANCK experiment over the dipole parameter is shown. The peaks shown in this figure arise from acoustic oscillations in the baryon-photon fluid as the photons decoupled from the thermal bath. During this period, gravitational wells formed from large amounts of dark matter. These gravitational wells pull the baryon-photon fluid inward, thereby compressing it. This process is counteracted by the pressure exerted by the photons, which leads to a rarefaction of the fluid. The temperature fluctuations of the CMB are then induced as the photons travel through different regions with varying gravitational potentials. Through the compression and rarefaction of

the baryon-photon fluid, oscillations are created. These oscillations are embedded in the power spectrum of the CMB, where the even-numbered peaks correspond to acoustic modes undergoing compression at the time of photon decoupling, while the odd-numbered peaks correspond to acoustic modes in a rarefaction phase. Through the amplitudes and positions of the peaks, we can now extract the cosmological parameters of the Λ CDM. The position of the first peak, which corresponds to the time of last scattering, allows us to infer the curvature of the universe. Further, the baryon content of the universe can be examined by taking the ratio of the amplitudes of the first and second peaks in the CMB power spectrum. This is motivated by the fact that if a higher baryon content exists in the baryon-photon fluid, this would result in a stronger compression and a weaker rarefaction. Vice versa, a smaller baryon density results in weaker compression and stronger rarefaction of the fluid. Analyzing, therefore, the amplitude ratios of the first two peaks allows us to obtain information on the baryon content in the universe. Furthermore, because dark matter does not interact with photons, it would only affect the amplitudes of the compression peaks. Therefore, a large third peak would indicate a sizeable dark matter content in the universe. The parameters of the base Λ CDM are used to fit the data points given in Fig. 3.1. Λ CDM consists of six independent parameters and assumes a flat universe ($k = 0$). The parameters and the measured values by Ref. [3] are the Hubble constant

$$H_0 = (67.4 \pm 0.5) \frac{\text{km}}{\text{s} \cdot \text{Mpc}}, \quad (3.20)$$

the baryon relic density

$$\Omega_b h^2 = 0.0224 \pm 0.0001, \quad (3.21)$$

the dark matter relic density

$$\Omega_c h^2 = 0.12 \pm 0.001, \quad (3.22)$$

the scalar spectral index

$$n_s = 0.965 \pm 0.004, \quad (3.23)$$

the matter fluctuation amplitude

$$\sigma_8 = 0.811 \pm 0.006, \quad (3.24)$$

and the optical depth

$$\tau = 0.054 \pm 0.007. \quad (3.25)$$

In Eqs. (3.21) and (3.22), the dimensional constant h is introduced, which reads

$$h^2 = \frac{H^2}{(100 \frac{\text{km}}{\text{sMpc}})^2}. \quad (3.26)$$

In order to compute the dark matter relic abundance $\Omega_c h^2$ for an arbitrary BSM theory, we need to first introduce the mathematical framework. We will discuss this in the next section.

3.5. Computation of the Dark Matter Relic Density

To obtain the relic density for a given model, the Boltzmann equation must be solved. In what follows, we will motivate this equation and provide a full derivation.

The Liouville operator

We start the derivation by introducing the Liouville equation [52],

$$L[f] = C[f] \quad , \quad (3.27)$$

where we introduced the functionals $L[f]$ and $C[f]$, which act on the phase space density f of an arbitrary particle species. The time evolution of the phase space density f is evaluated with Eq. (3.27). At the end of this derivation, we will obtain from this function an equation that describes the time evolution of the particle number density n .

First, we will focus on the LHS. In the general relativistic limit, $L[f]$ is given by

$$L[f] = \frac{df}{d\tau} = p^\mu \frac{\partial f}{\partial x^\mu} + \frac{dp^\mu}{d\tau} \frac{\partial f}{\partial p^\mu} \quad , \quad (3.28)$$

where τ is the proper time, x_μ the space time four-vector and

$$p_\mu = \frac{dx_\mu}{d\tau} = \begin{pmatrix} E \\ \mathbf{p} \end{pmatrix} \quad (3.29)$$

the four-momentum, where E is the energy and $\mathbf{p}$ is the three-momentum of a particle with mass m . We can now use the geodesic equation [52]

$$\frac{dp^\mu}{d\tau} = -\Gamma_{\alpha\beta}^\mu p^\alpha p^\beta \quad , \quad (3.30)$$

where $\Gamma_{\alpha\beta}^\mu$ are the Christoffel symbols, to rewrite the second term of Eq. (3.28). This leads to the following form

$$L[f] = p^\mu \frac{\partial f}{\partial x^\mu} - \Gamma_{\alpha\beta}^\mu p^\alpha p^\beta \frac{\partial f}{\partial p^\mu} \quad . \quad (3.31)$$

Boltzmann equation

With the assumption that our universe is homogeneous and isotropic [54], the phase-space density is only dependent on the energy E and the time t . This simplifies Eq. (3.31) to

$$L[f] = E \frac{df}{dt} - \Gamma_{\alpha\beta}^\mu p^\alpha p^\beta \frac{\partial f}{\partial p^\mu} \quad . \quad (3.32)$$

The Christoffel symbols are defined as

$$\Gamma_{\alpha\beta}^\mu = \frac{1}{2} g^{\mu\lambda} \left(\frac{\partial g_{\beta\lambda}}{\partial x^\alpha} + \frac{\partial g_{\alpha\lambda}}{\partial x^\beta} - \frac{\partial g_{\alpha\beta}}{\partial x^\lambda} \right) \quad , \quad (3.33)$$

where the metric $g_{\mu\nu}$ is given by

$$g_{\mu\nu} = \begin{cases} 1, & \text{for } \mu = \nu = 0 \\ -a(t)^2, & \text{for } \mu = \nu \in (1, 2, 3) \\ 0, & \text{for } \mu \neq \nu \end{cases} \quad . \quad (3.34)$$

$$g_{\mu\nu} = \begin{cases} 1, & \text{for } \mu = \nu = 0 \\ -a(t)^2, & \text{for } \mu = \nu \in (1, 2, 3) \\ 0, & \text{for } \mu \neq \nu \end{cases} \quad (3.35)$$

$$g_{\mu\nu} = \begin{cases} 1, & \text{for } \mu = \nu = 0 \\ -a(t)^2, & \text{for } \mu = \nu \in (1, 2, 3) \\ 0, & \text{for } \mu \neq \nu \end{cases} \quad (3.36)$$

With the metric specified, we observe that only the Γ_{ij}^0 components with $(i, j \in \{1, 2, 3\})$ are non-zero. These components are explicitly given by

$$\Gamma_{ij}^0 = \dot{a}(t) a(t) \delta_{ij} \quad . \quad (3.37)$$

Next, we define an expression for p_i . The square of the four-momentum has to fulfill the following equation [5]

$$g_{\mu\nu}p^\mu p^\nu = m^2 = E^2 - \mathbf{p}^2 . \quad (3.38)$$

From this relation, the components of the three-momentum ($i, j \in \{1, 2, 3\}$) can be identified as

$$\mathbf{p}^2 = -g_{ij}p^i p^j \rightarrow p^i = \frac{|\mathbf{p}|}{a} \hat{e}^i . \quad (3.39)$$

By substituting Eqs. (3.37) and (3.39) into Eq. (3.32), we obtain

$$L[f] = E \frac{df}{dt} - H|\mathbf{p}|^2 \frac{\partial f}{\partial E} . \quad (3.40)$$

Next, we multiply Eq. (3.40) with $\frac{d^3p \cdot g}{(2\pi)^3}$ and integrate over d^3p . In the multiplicative factor, we introduced the spin degrees of freedom g of the particle. The first term is evaluated by introducing the particle number density n , which is given by

$$n = g \int \frac{d^3p}{(2\pi)^3} f . \quad (3.41)$$

Using this equation, the first term of Eq. (3.40) is then given by

$$g \int \frac{d^3p}{(2\pi)^3} E \frac{df}{dt} = gE \frac{d}{dt} \int \frac{d^3p}{(2\pi)^3} f = E \frac{dn}{dt} . \quad (3.42)$$

The second term of Eq. (3.40) can also be evaluated by performing a change in variables given by

$$\frac{\partial f}{\partial E} = \frac{\partial f}{\partial p} \frac{E}{|\mathbf{p}|} ,$$

and also integrating by parts, which leads to the following form

$$-Hg \int \frac{d^3p}{(2\pi)^3} |\mathbf{p}|^2 \frac{\partial f}{\partial E} = -HgE \int \frac{dp d\Omega}{(2\pi)^3} |\mathbf{p}|^3 \frac{\partial f}{\partial p} = HgE \int \frac{dp d\Omega}{(2\pi)^3} f \frac{\partial |\mathbf{p}|^3}{\partial p} = 3HEn . \quad (3.43)$$

Combining now Eqs. (3.40), (3.42) and (3.43), we finally arrive at the Boltzmann equation [60]

$$\frac{dn}{dt} + 3Hn = g \int \frac{d^3p}{(2\pi)^3} \frac{C[f]}{E} \quad (3.44)$$

In the next section, we will focus on the right-hand side. We will see that the explicit form of the collision operator $C[f]$ depends on the thermal production mechanism we assume. In the following sections, we will introduce the thermal production mechanism which is assumed to produce dark matter in this thesis, the freeze-out mechanism [61]. We will describe the freeze-out mechanism following the description of Ref. [60].

Thermal Freeze-Out

In this production mechanism, we assume that in the early Universe every particle, including the dark matter particle, is in thermal equilibrium with the thermal bath. This implies that the production and annihilation rates are equal. However, due to the expansion of the Universe, two effects occur, which we briefly explain below.

1. As the Universe expands, the temperature T decreases. Consequently, light particles no longer have enough energy to efficiently produce heavy particles. The annihilation process then becomes dominant, and the heavy particle number density decreases.
2. Due to the expansion of the Universe, it also becomes less likely for two particles to interact. As a result, the annihilation rate Γ_{ann} decreases. When the annihilation rate becomes comparable to the expansion rate of the Universe, i.e. $\Gamma_{\text{ann}} = H$, annihilations cease to be efficient. This point in time is referred to as freeze-out point.

For the sake of simplicity, we will focus on $2 \rightarrow 2$ processes of the form $1 + 2 \rightarrow 3 + 4$. The integrated collision operator in Eq.(3.44) reads

$$g \int \frac{d^3p}{(2\pi)^3} \frac{C[f]}{E} = - \sum_{\text{spin}} \int \prod_{i=1}^4 d\Pi_i \left[f_1 f_2 (1 \pm f_3)(1 \pm f_4) |\mathcal{M}_{12 \rightarrow 34}|^2 \right. \\ \left. - f_3 f_4 (1 \pm f_1)(1 \pm f_2) |\mathcal{M}_{34 \rightarrow 12}|^2 \right] (2\pi)^4 \delta^{(4)}(p_1 + p_2 - p_3 - p_4) \quad . \quad (3.45)$$

Here we defined the phase space measure

$$d\Pi_i \equiv \frac{d^3p_i}{(2\pi)^3 2E_i} \quad , \quad (3.46)$$

for an arbitrary particle $i \in 1, 2, 3, 4$ with energy E_i . In Eq.(3.45), $|\mathcal{M}_{ij \rightarrow kl}|^2$ denotes the squared matrix element of the process $ij \rightarrow kl$. The $(1 \pm f_i)$ terms represents Pauli blocking ($-$) or Bose enhancement. Fermions cannot occupy the same state, while bosons are able to do so. One can simplify Eq. 3.45 further by applying the following assumptions [62],

1. As all bath particles are in thermal equilibrium, one can write through detailed balance the following equation

$$f_3 f_4 = f_3^{\text{eq}} f_4^{\text{eq}} = f_1^{\text{eq}} f_2^{\text{eq}} \quad , \quad (3.47)$$

where f_i^{eq} ($i \in [1, 2, 3, 4]$) denotes the phase space density of particle i in thermal equilibrium.

2. As the phase space density f_i is $f_i \ll 1$, the $(1 \pm f_i)$ terms can be replaced by 1.

3. Because of unitarity, we can write the

$$\sum_{\text{spin}} \int d\Pi_3 d\Pi_4 (2\pi)^4 \delta^4(p_1 + p_2 - p_3 - p_4) |\mathcal{M}|_{12 \rightarrow 34}^2 = \\ \sum_{\text{spin}} \int d\Pi_3 d\Pi_4 (2\pi)^4 \delta^4(p_1 + p_2 - p_3 - p_4) |\mathcal{M}|_{34 \rightarrow 12}^2 \quad . \quad (3.48)$$

Using the relation for the cross section $\sigma_{12 \rightarrow 34}$, which is given by

$$\sigma_{12 \rightarrow 34} = \sum_{\text{spin}} \int \frac{d^3p_3}{(2\pi)^3 2E_3} \frac{d^3p_4}{(2\pi)^3 2E_4} \frac{|\mathcal{M}|_{12 \rightarrow 34}^2 (2\pi)^4 \delta^{(4)}(p_1 + p_2 - p_3 - p_4)}{4g_1 g_2 \sqrt{(p_1 \cdot p_2) - m_1^2 m_2^2}}, \quad (3.49)$$

where we m_i and g_i ($i \in [1, 2]$) are the masses and the spin degrees of freedom of the initial state particles, we can further simplify the Expression in Eq. (3.45). Furthermore, we sum

up all cross sections for all possible final state configurations, such that we introduce the following relation

$$\sigma = \sum_f \sigma_{12 \rightarrow f} \quad . \quad (3.50)$$

Applying these assumptions, the collision operator is then given by

$$g \int \frac{d^3 p}{(2\pi)^3} \frac{C[f]}{E} = -g_1 g_2 \int \sigma v_{\text{Møl}} (f_1 f_2 - f_1^{\text{eq}} f_2^{\text{eq}}) \frac{d^3 p_1}{(2\pi)^3} \frac{d^3 p_2}{(2\pi)^3} \quad (3.51)$$

where

$$v_{\text{Møl}} = \frac{\sqrt{(p_1 \cdot p_2) - m_1^2 m_2^2}}{E_1 E_2} \equiv v \quad , \quad (3.52)$$

is the Møller velocity. To evaluate how dark matter particles depart from thermal equilibrium, we need to define what this means. A particle in thermal equilibrium is in both chemical and thermal equilibrium. Chemical equilibrium means its number density matches the equilibrium density. Kinetic equilibrium ensures the energy dependence of the distribution function matches that in equilibrium. Thus, for an arbitrary particle i , the distribution function $f_i(E, t)$ reads

$$f_i = \chi_i(t) f_i^{\text{eq}}(E), \quad (3.53)$$

where $\chi_i(t)$ is some function, which depends on the time t [63]. Next, the thermal average of an operator $\mathcal{O}(p_1, p_2)$ is given by

$$\langle \mathcal{O} \rangle = \frac{1}{n_1^{\text{eq}} n_2^{\text{eq}}} \int \frac{d^3 p_1}{(2\pi)^3} \frac{d^3 p_2}{(2\pi)^3} g_1 g_2 f_1^{\text{eq}} f_2^{\text{eq}} \mathcal{O}(p_1, p_2) \quad . \quad (3.54)$$

Using Eqs. (3.53) and (3.54), we can rewrite Eq. (3.51) such that we obtain

$$g \int \frac{d^3 p}{(2\pi)^3} \frac{C[f]}{E} = -\langle \sigma v \rangle (n_1 n_2 - n_1^{\text{eq}} n_2^{\text{eq}}) \equiv -\langle \sigma v \rangle (n^2 - n_{\text{eq}}^2) \quad , \quad (3.55)$$

where we used the assumption that the number density of particles 1 and 2 are the same, such that

$$n_1 = n_2 \equiv n \quad . \quad (3.56)$$

Finally combining Eqs. (3.44) and (3.55), we arrive at the Boltzmann equation, which reads

$$\frac{dn}{dt} + 3Hn = -\langle \sigma v \rangle (n^2 - n_{\text{eq}}^2) \quad (3.57)$$

In order to cancel the effects of the expansion of the universe on the number density of the particle, we introduce a new quantity called the yield Y , which is given by

$$Y = \frac{n}{s} \quad , \quad (3.58)$$

where s denotes the entropy density of the universe. Assuming that the entropy $S = a^3 s$ is constant in time, we can write the time derivative of Eq. (3.58) as

$$\frac{dY}{dt} = \frac{1}{s} \frac{dn}{dt} + 3H \frac{n}{s} \quad , \quad (3.59)$$

where we used that

$$\frac{ds}{dt} = -3 \frac{1}{a} \frac{da}{dt} s = -3Hs \quad . \quad (3.60)$$

We then can rewrite Eq. (3.57) as

$$\frac{dY}{dt} = -s\langle\sigma v\rangle(Y^2 - Y_{\text{eq}}^2). \quad (3.61)$$

Next, we perform a variable transformation from the time t to the temperature T dependent variable $x = \frac{m_\chi}{T}$, where m_χ denotes the dark matter particles. Using this variable transformation, Eq. (3.61) reads

$$\frac{dY}{dx} = -\frac{m_\chi}{x^2} \frac{1}{3H} \frac{ds}{dT} \langle\sigma v\rangle (Y^2 - Y_{\text{eq}}^2). \quad (3.62)$$

Here, we used the following relation

$$\left(\frac{dT}{dt}\right)^{-1} = \left(\frac{ds}{dT}\right)^{-1} \frac{ds}{dT} = -\frac{1}{3Hs} \frac{ds}{dT}. \quad (3.63)$$

The Friedmann equation in a radiation-dominated universe is given by

$$H^2 = \frac{8\pi\rho G}{3}, \quad (3.64)$$

denotes G denote the gravitational constant, and ρ is the energy density. We can write both the energy density ρ and entropy density in terms of the effective degrees of freedom g_{eff} and h_{eff} , respectively, such that they read

$$\rho = g_{\text{eff}}(T) \frac{\pi^2}{30} T^4 \quad s = h_{\text{eff}}(T) \frac{2\pi^2}{45} T^3. \quad (3.65)$$

Equation (3.62) can then be written as

$$\frac{dY}{dx} = -\sqrt{\frac{\pi}{45G}} \langle\sigma v\rangle \frac{g_{1/2}^* m_\chi}{x^2} (Y^2 - Y_{\text{eq}}^2), \quad (3.66)$$

where we introduced $g_*^{1/2}$ as

$$g_{1/2}^* = \frac{h_{\text{eff}}}{g_{\text{eff}}^{1/2}} \left(1 + \frac{T}{3h_{\text{eff}}} \frac{dh_{\text{eff}}}{dT}\right). \quad (3.67)$$

To obtain the relic density now, one needs to solve Eq. (3.66) from $x = 0$ to $x_0 = m_\chi/T_0$, where T_0 denotes the temperature of the universe today [3],

$$T_0 = (2.7255 \pm 0.0006) \text{ K}, \quad (3.68)$$

with the initial condition $Y(0) = Y_{\text{eq}}(0)$. By solving Eq. (3.66), we obtain the current yield Y_0 today, so we can use Eq. (3.12), to obtain dark matter relic density

$$\Omega_\chi h^2 = \frac{m_\chi Y_0 s_0}{3M_{\text{PL}} H_0^2} h^2 \approx 2.742 \frac{m_\chi}{\text{GeV}} Y_0. \quad (3.69)$$

3.6. Direct Detection

The basic idea of directly detecting dark matter was first proposed in Ref. [64]. The dark matter candidate can interact with the SM particles via a mediator particle. Therefore, there is an effective dark matter-nucleus interaction. Therefore, dark matter can scatter with some nuclei. The recoil energy could be measured, providing direct evidence for weakly interacting

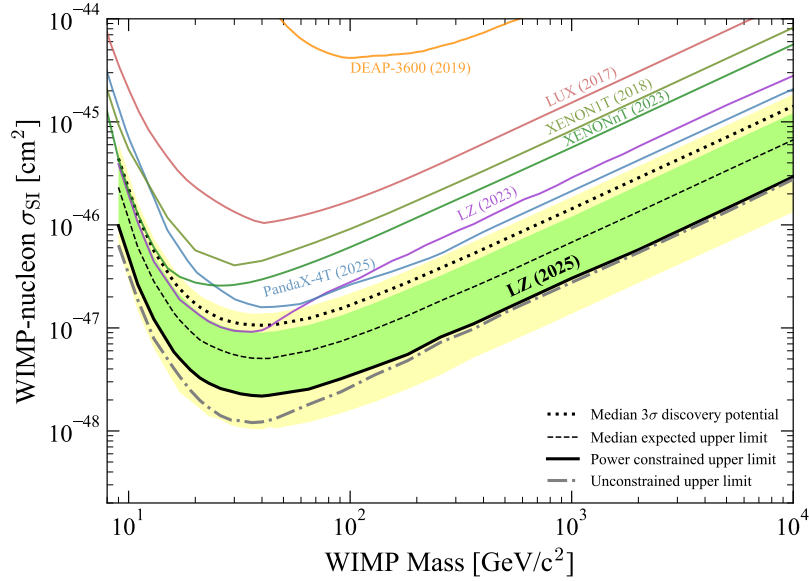


Figure 3.2.: Exclusion limit of the spin-independent DD-cross-section over the WIMP dark matter mass obtained by the *Lux-Zeplin* experiment. Taken from [4].

dark matter. At the time of this work, current direct-detection (DD) searches [4] have not observed any signals. Nonetheless, these experiments can be used to set exclusion bounds on dark matter models. In Fig. 3.2, we show the current exclusion limits set by the *Lux-Zeplin* experiment. It can be seen that there is still parameter space remaining, allowing for dark matter signals in DD experiments. To compare the theoretical prediction with the experiment, we first need to establish the theoretical framework, which we describe below. The differential scattering rate dR per energy interval dE reads [65]

$$\frac{dR}{dE} = \sum_i k_i \frac{\sigma_i}{2m_\chi \mu_i} \rho_0 \eta_i, \quad (3.70)$$

where k_i denotes the mass fraction of the nucleon i in the detector, σ_i the dark matter-nucleus scattering cross section, ρ_0 the local dark matter density and μ_i is the reduced mass, which reads

$$\mu_i = \frac{m_\chi m_i}{m_\chi + m_i}. \quad (3.71)$$

Here, m_i denotes the nucleon mass and m_χ the mass of the dark matter particle χ . The variable η_i is a function of the local velocity distribution $f(\vec{v})$ of the dark matter particle relative to the detector. It reads

$$\eta_i = \int_{v_{\min,i}}^{v_{\text{esc}}} d^3v \frac{f(\vec{v})}{v}. \quad (3.72)$$

Here, $v_{\min,i}$ denotes the minimal velocity which induces a recoil energy E in the detector,

$$v_{\min,i} = \frac{m_i E}{2\mu_i}, \quad (3.73)$$

and v_{esc} denotes the galactic escape velocity. The typical velocity is of order $10^{-3}c$. We assume that the nuclei in the detector are at rest, which means that the typical recoil energy, which is proportional to the momentum transfer q , is of order 1–100 keV. In light of this small energy exchange, compared to the rest mass of the nuclei, we assume a vanishing momentum transfer, i.e., $q^2 \rightarrow 0$. In the dark matter-nucleus scattering cross section, all information

on the dark matter-nucleus interaction is encoded. In the limit, where $q^2 \rightarrow 0$, the only contributions that enter the cross section are from spin-independent (SI) and spin-dependent (SD) interactions. To compare results across experiments, one usually expresses them in terms of the scattering cross section for a single nucleon-dark matter particle interaction. To describe the dark matter-nucleon interaction, the effective field theory (EFT) approach is used. At low energies, the dark matter-nucleon scattering can be described as an effective four-fermion interaction. These interactions are parametrized in terms of effective operators. The effective Lagrangian of the dark matter-quark interaction is given by

$$\begin{aligned}\mathcal{L}_{\chi q}^{\text{EFT}} &= c_s \mathcal{O}_s + c_V \mathcal{O}_V + c_A \mathcal{O}_A + c_T \mathcal{O}_T \\ &= c_s [\bar{\chi} \chi \bar{q} q] + c_V [\bar{\chi} \gamma^\mu \chi \bar{q} \gamma_\mu q] + c_A [\bar{\chi} \gamma^\mu \gamma_5 \chi \bar{q} \gamma_\mu \gamma_5 q] - \frac{1}{2} c_T [\bar{\chi} \sigma^{\mu\nu} \chi \bar{q} \sigma_{\mu\nu} q],\end{aligned}\quad (3.74)$$

where $c_i \equiv c_{i,q}$ ($i \in [s, V, A, T]$) denote the Wilson coefficients, which in general depend on the quark flavour q , and $\sigma_{\mu\nu}$ is given by

$$\sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu]. \quad (3.75)$$

The effective six-dimensional operators $\mathcal{O}_i$ denote the scalar, vector, axial-vector, and tensor interactions between four fermions. In general, there are more operators; however, they are velocity-dependent and, therefore, for our purposes, omitted. Within the discussed limit, the SI contributions are given by scalar and vector interactions, while the SD contributions are induced by axial-vector and tensor interactions. After defining the dark matter-quark interactions, we now need to translate them into nucleon interactions. Considering the dark matter-nucleon interaction, the effective Lagrangian is given by replacing q in Eq. (3.74) by the nucleon $N = \{p, n\}$ such that it reads

$$\begin{aligned}\mathcal{L}_{\chi N}^{\text{EFT}} &= c_{s,N} [\bar{\chi} \chi \bar{N} N] + c_{V,N} [\bar{\chi} \gamma^\mu \chi \bar{N} \gamma_\mu N] + c_{A,N} [\bar{\chi} \gamma^\mu \gamma_5 \chi \bar{N} \gamma_\mu \gamma_5 N] \\ &\quad - \frac{1}{2} c_{T,N} [\bar{\chi} \sigma^{\mu\nu} \chi \bar{N} \sigma_{\mu\nu} N].\end{aligned}\quad (3.76)$$

In what follows, we consider only the SI contributions and omit the SD contributions. The first matrix element is the scalar current, which is interpreted as the contribution of the quark mass m_q to the nucleon mass m_N . It reads

$$\langle N | m_q \bar{q} q | N \rangle = m_N f_q^N, \quad (3.77)$$

where the form factors f_N^q are obtained on the lattice. In Tab. 3.1, we provide the numerical values of the form factors. Equation (3.77) is valid for light quarks, i.e., $q = \{u, d, s\}$. The interactions of heavy quarks are redefined as a dark matter-Gluon interaction via a heavy quark loop. The corresponding matrix element for this interaction is given by

$$\begin{aligned}\langle N | m_Q \bar{Q} Q | N \rangle &= -\frac{\alpha_S}{12\pi} \langle N | G_{\mu\nu}^i G^{i,\mu\nu} | N \rangle = -\frac{\alpha_S}{12\pi} \left(-\frac{8\pi}{9\alpha_S} \right) m_N \left(1 - \sum_{q=u,d,s} f_q^N \right) \\ &= \frac{2}{27} m_N \left(1 - \sum_{q=u,d,s} f_q^N \right).\end{aligned}\quad (3.78)$$

Here, α_S denotes the strong coupling constant, and $G^{i,\mu\nu}$ ($i \in [1, \dots, 8]$) are the gluonic field strength tensor. We can now express the scalar Wilson coefficient $c_{s,N}$ of the effective dark matter-nucleon Lagrangian in terms of the Wilson coefficients $c_{s,q}$ of the dark matter-quark Lagrangian as follows

$$c_{s,N} = m_N \left(\sum_{q=u,d,s} f_q^N \frac{c_{s,q}}{m_q} + \frac{2}{27} \left(1 - \sum_{q=u,d,s} f_q^N \right) \sum_{q=c,b,t} \frac{c_{s,q}}{m_q} \right). \quad (3.79)$$

	u	d	s
f_q^p	0.0153	0.0191	0.0447
f_q^n	0.011	0.0273	0.0447

Table 3.1.: Form factors for the proton f_q^p and the neutron f_q^n for $q = u, d, s$. Values Taken from [66].

The matrix element of the vector current can be interpreted as the number of valence quarks in a nucleon. It therefore reads

$$\langle N | m_q \bar{q} \gamma_\mu q | N \rangle = n_q^N, \quad (3.80)$$

where $n_u^n = 1$, $n_d^n = 2$ and $n_u^p = 2$, $n_d^p = 1$. The vector dark matter-nucleon Wilson coefficient $c_{V,N}$ then reads

$$c_{V,N} = \sum_{u,d} n_q^N \frac{c_{V,q}}{m_q}. \quad (3.81)$$

The SI cross section for the dark matter-nucleon scattering is then given by [65]

$$\sigma_{\text{SI}} = \frac{4\mu_\chi}{\pi} \left[\frac{c_{s,p} \pm c_{V,p}}{2} Z + \frac{c_{s,n} \pm c_{V,n}}{2} (A - Z) \right]^2. \quad (3.82)$$

where Z is the proton number and A is the atomic number. The $+$ ($-$) sign denotes the dark matter (anti-dark matter) interaction, and the reduced mass μ_χ reads

$$\mu_\chi = \frac{m_N m_\chi}{m_N + m_\chi} \quad (3.83)$$

In the case of where the dark matter particle is its own anti-particle, the Wilson coefficients become

$$\frac{c_{s,N} \pm c_{V,N}}{2} \rightarrow c_{s,N}, \quad (3.84)$$

which then translates to the following SI cross section

$$\sigma_{\text{SI}}^{\text{real}} = \frac{4\mu_\chi}{\pi} [c_{s,p} Z + c_{s,n} (A - Z)]^2. \quad (3.85)$$

Part II.

Investigation of CP-Violation in the Complex Two-Higgs-Doublet Model

To make predictions across different BSM models, it is important to understand how constraints affect the parameter space. In this part, we will investigate how collider constraints and the electron electric dipole moment (eEDM) constraint interplay in the C2HDM framework, which we introduced in Sec. 2.3.

We work in a CP-violating 2HDM with a softly broken $\mathbb{Z}_2$ symmetry that allows CP violation both in the scalar potential and the Higgs Yukawa interaction. The model naturally eliminates FCNC at tree level while still accommodating CP violation, thereby generating EDMs for fundamental particles. The dominant contributions of the EDM are given by the two-loop Barr-Zee diagrams [67]. Further, it has been seen in Ref. [41] that a new type of two-loop diagrams, dubbed as "kite diagrams", are necessary to obtain a gauge-independent result. In recent developments [68], it has also been shown that one-loop diagrams are relevant to the calculation of the eEDM. There are two reasons why it is important to keep track of the relevant diagrams when calculating the eEDM. First, the experimental sensitivity is steadily improving: the current 90% confidence-level limit given by the ACME collaboration is $1.1 \times 10^{-29} \text{e.cm}$ [69–71], while the JILA collaboration sets a limit of $4.1 \times 10^{-30} \text{e.cm}$ [71]. However, the individual contributions to the eEDM are of order 10^{-27} . This means that there must be a large cancellation among the eEDM diagrams to obtain a significant CP violation, while still accommodating the eEDM constraints. In prospect of the expected future sensitivity of $\mathcal{O}(10^{-33})$ [72–74], formerly neglected diagrams become more and more relevant. We also show that virtual charm quarks must be considered in the Barr-Zee diagrams to obey the expected sensitivity.

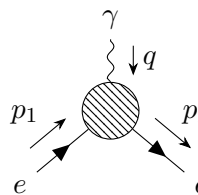
Our approach will be as follows. We will perform an extensive parameter scan in the Type II of the C2HDM with $h_2 = h_{125}$, where h_{125} represents the SM-like Higgs boson. Here, we apply all theoretical and experimental constraints to obtain a valid parameter set. We will use two scan methods in our analysis, the guided scan and a scan using Machine Learning (ML) algorithms. These scans are then used to quantify the allowed size of CP violation in the fermionic couplings to the SM-like Higgs boson, in light of additional contributions to the EDM calculation and the most recent experimental data.

In this chapter, we present the formulas used to compute the electron EDM. Then we will provide the list of theoretical and experimental constraints applied, along with the scan ranges for the input parameters.

4.1. Electron Electric Dipole Moment

The calculation of the electric dipole moment has been developed since 1990, first done by Barr and Zee [67]. In the first calculation, the two-loop Barr-Zee diagrams were considered, which were followed by further extensions [75–77]. However, this calculation was not gauge-invariant, as the calculation only consisted of a leading subset of all two-loop contributions to the EDM. In recent work [41], it has been shown that including kite diagrams yields gauge-invariant results. In this section, we will provide the formulas used to calculate the electron EDM. We will follow the description⁸ given in Ref. [41], where the complete two-loop calculation has been done.

The electron EDM d_e is obtained from the CP-odd Pauli form factor in the electromagnetic vertex in the limit of $q^2 = 0$, where q denotes the four-momentum of the outgoing photon. The form factor is given by



$$\text{Diagram} \supset id_e \bar{u}(p_1) \sigma^{\mu\nu} q_\nu \gamma_5 u(p_2), \quad (4.1)$$

where γ_5 is given in terms of the Dirac matrices γ^μ ($\mu \in [0, 1, 2, 3]$)

$$\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3, \quad (4.2)$$

$\sigma^{\mu\nu}$ reads as

$$\sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu], \quad (4.3)$$

and u denotes the spinor of the electron (positron). The eEDM d_e is then given by

$$\frac{d_e}{e} = \frac{\sqrt{2}\alpha(\mu)G_F m_e}{64\pi^3} \delta_e. \quad (4.4)$$

Here, m_e denotes the electron mass, G_F denotes the Fermi constant, α the fine structure constant at the scale μ . Here, we evaluate the fine-structure constant at the Thompson limit $\mu = 0$. We will present the different contributions in terms of the dimensionless electric dipole moment δ_e . These contributions are evaluated with the background field method (BFM) gauge.⁹

In Tab. 4.1, we show the two-loop contributions of the eEDM in the C2HDM. The Barr-Zee diagrams constitute the largest group numbers in the eEDM calculation. The remaining diagrams are the kite diagrams, which are fewer in number than the Barr-Zee diagrams. They are formally of the same order as the Barr-Zee diagrams and are essential to obtain a gauge-independent result. For the results given in the next subsections, we employ the following shorthand notation of the squared mass ratios with respect to the mass squared of the k -th ($k \in [1, 2, 3]$) neutral Higgs,

$$r_k = \frac{m_f^2}{m_k^2}, \quad w_k = \frac{m_W^2}{m_k^2}, \quad z_k = \frac{m_Z^2}{m_k^2}, \quad h_k = \frac{m_{H^\pm}^2}{m_k^2}. \quad (4.5)$$

⁸In our analysis, we use the expressions for the Barr-Zee diagrams given in Ref. [78]. We have explicitly verified that these results agree numerically with those presented in Ref. [41]. For consistency, we therefore adopt the formulation of Ref. [41] throughout.

⁹Note that it has been shown in Ref. [41] that one also obtains a gauge-independent result in the R_ξ gauge. Re-evaluating these results in the R_ξ gauge, however, is beyond the scope of this work, and we refer to Ref. [41].

Barr-Zee	Fermion loop	Charged Higgs loop	Gauge boson loop
Electromagnetic	δ_f^{EM}	$\delta_{H^\pm}^{\text{EM}}$	$\delta_W^{\text{EM}}(\xi)$
Neutral current	δ_f^{NC}	$\delta_{H^\pm}^{\text{NC}}$	$\delta_W^{\text{NC}}(\xi)$
Charged current	0	$\delta_{H^\pm}^{\text{CC}}$	$\delta_W^{\text{CC}}(\xi)$
Kite			
Neutral Current	0	0	$\delta_{\text{kite}}^{\text{NC}}$
Charged Current	0	0	$\delta_{\text{kite}}^{\text{CC}}(\xi)$

Table 4.1.: Two-loop contributions to the eEDM in the C2HDM. The rows indicate the couplings to the main fermion line, while the columns indicate the virtual particles in the loop. The input parameter ξ denotes the gauge parameter. Taken from Ref. [41].

Furthermore, we introduce the Davydchjev-Tausk vacuum integral function [79], which reads

$$\begin{aligned} \Phi(x, y) = & \text{Re} \left\{ \frac{2}{\sqrt{\lambda}} \left(\frac{\pi^2}{6} - \frac{1}{2} \ln x \ln y + \ln \left(\frac{1+x-y-\sqrt{\lambda}}{2} \right) \ln \left(\frac{1-x+y-\sqrt{\lambda}}{2} \right) \right) \right\} \\ & - \text{Re} \left\{ \frac{2}{\sqrt{\lambda}} \left(\text{Li}_2 \left(\frac{1+x-y-\sqrt{\lambda}}{2} \right) + \text{Li}_2 \left(\frac{1-x+y-\sqrt{\lambda}}{2} \right) \right) \right\}, \end{aligned} \quad (4.6)$$

where $\text{Li}_2(x)$ is the Spence function and λ is the Källén function, which reads

$$\lambda = (1-x-y)^2 - 4xy. \quad (4.7)$$

In the case, when $y = x$, Eq. (4.6) simplifies to

$$\Phi(x) \equiv \Phi(x, x) = \frac{2}{\sqrt{1-4x}} \left[\frac{\pi^2}{6} + \ln^2 \frac{1-\sqrt{1-4x}}{2} - \frac{\ln^2 x}{2} - 2\text{Li}_2 \left(\frac{1-\sqrt{1-4x}}{2} \right) \right]. \quad (4.8)$$

Fermion Loop Contributions

First, we present the expressions used for the diagrams, in which the virtual particles are fermions, i.e., those listed in the first column of Tab. 4.1. The corresponding diagram is shown in Fig. 4.1. To obtain an exact prediction for the EDM, all fermions in the loops must be included. However, since the diagrams are proportional to the fermion masses, contributions from light fermions are strongly suppressed compared to those from third-generation fermions. In our work, we consider the third-generation fermions and also include the charm quark in the calculation. The Barr-Zee diagrams with a photon propagator give the following contribution

$$\begin{aligned} \delta_f^{\text{EM}} = & -4N_C^f (Q_{\text{EM}}^f)^2 Q_{\text{EM}}^l \sum_k \text{Im}(q_{k2}) \left\{ c_f \left(q_{k1} - 2T_3^l c_l \text{Re}(q_{k2}) \right) r_k \Phi(r_k) \right. \\ & \left. + \left(q_{k1} - 2T_3^f c_f \text{Re}(q_{k2}) \right) c_l r_k \left[4 + 2 \ln r_k + (1 - 2r_k) \Phi(r_k) \right] \right\} \end{aligned} \quad (4.9)$$

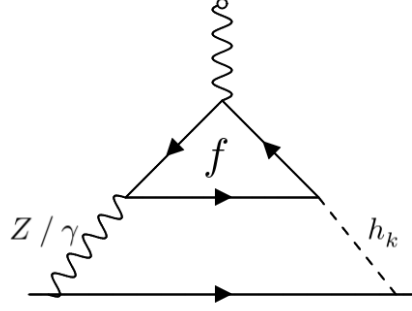


Figure 4.1.: Generic diagram of the fermion loop contribution of the electromagnetic and neutral Barr-Zee diagrams. The white dot represents the background field $\bar{A}_\mu$.

Here, $N_C^f = 3(1)$ for quarks (leptons) and Q_{EM}^f and T_3^f are the electric charge and the third component of the weak isospin, respectively. Also, the matrix elements q_{ij} are given in Eq. (2.58). The EDM contribution of the diagrams with a Z boson propagator is given by

$$\begin{aligned} \delta_f^{\text{NC}} = & -\frac{N_C^f Q_{\text{EM}}^f Q_W^f Q_W^l}{4 \cos^2 \theta_W \sin^2 \theta_W} \sum_k \text{Im}(q_{k2}) \left\{ c_f \left(q_{k1} - 2T_3^l c_l \text{Re}(q_{k2}) \right) \frac{r_k}{1 - z_k} \left[\Phi(r_k) - \Phi\left(\frac{r_k}{z_k}\right) \right] \right. \\ & \left. + \left(q_{k1} - 2T_3^f c_f \text{Re}(q_{k2}) \right) c_l \frac{r_k}{1 - z_k} \left[2 \ln z_k + (1 - 2r_k) \Phi(r_k) - \left(1 - \frac{2r_k}{z_k} \right) \Phi\left(\frac{r_k}{z_k}\right) \right] \right\}, \end{aligned} \quad (4.10)$$

where θ_W denotes the weak mixing angle and Q_W^f denotes the weak charge of a fermion f and c_f ($f \in [l, u, d]$) denotes the coupling modifier defined in Sec. 2.3. Note that contributions involving fermion loops are all gauge-independent.

Charged Higgs Loop Contributions

The charged Higgs contributions have three types of Barr-Zee diagrams. In Fig. 4.2, the electromagnetic and neutral-charged Barr-Zee diagrams are shown in the top row, while the charged-current Barr-Zee diagrams are shown in the bottom row. Like the fermion contributions, the charged Higgs loops are, also gauge-independent, as expected. The electromagnetic charged Higgs contribution is given by

$$\delta_{H^\pm}^{\text{EM}} = \frac{2Q_{\text{EM}}^l \sin^2 \theta_W}{\pi \alpha} c_l \sum_k \text{Im}(q_{k2}) \lambda_{kH^+H^-} w_k [2 + \ln h_k - h_k \Phi(h_k)]. \quad (4.11)$$

Here, $\lambda_{kH^+H^-}$ represents the trilinear coupling between H_k and the charged Higgs bosons $H^\pm$. Next, the neutral current charged Higgs contribution is given by

$$\delta_{H^\pm}^{\text{NC}} = \frac{Q_W^l \cos 2\theta_W}{4\pi \alpha} c_l \sum_k \text{Im}(q_{k2}) \lambda_{kH^+H^-} \frac{z_k}{1 - z_k} \left[\ln z_k - h_k \Phi(h_k) + \frac{h_k}{z_k} \Phi\left(\frac{h_k}{z_k}\right) \right]. \quad (4.12)$$

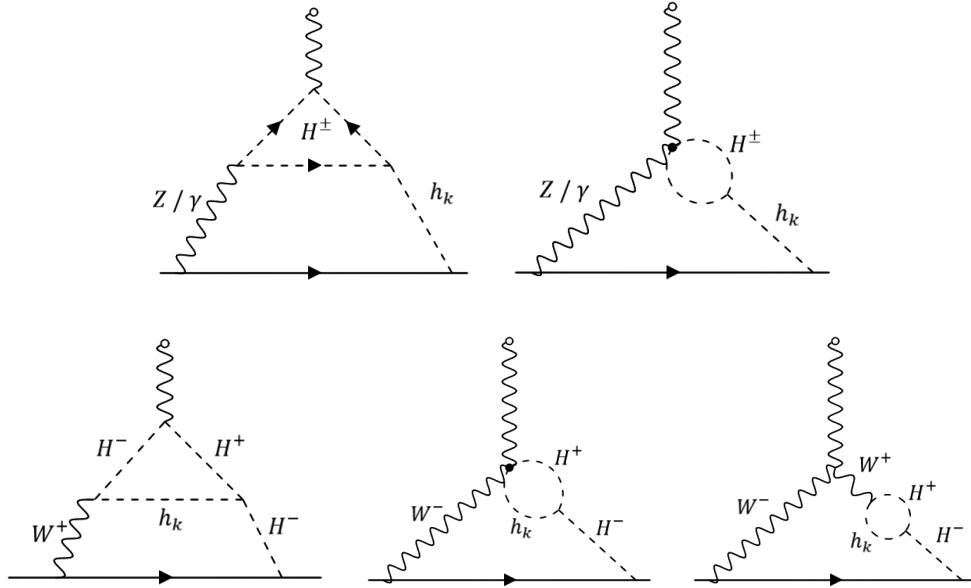


Figure 4.2.: Generic diagrams from the contributions with charged Higgs bosons in the loop. The white dot represents the background field $\bar{A}_\mu$. Top row: electromagnetic and neutral current contributions $\delta_{H^\pm}^{\text{EM}}$ and $\delta_{H^\pm}^{\text{NC}}$. Bottom row: charged current contributions $\delta_{H^\pm}^{\text{CC}}$.

Lastly, the contributions of the charged current charged Higgs Barr-Zee diagrams are given by

$$\delta_{H^\pm}^{\text{CC}} = \frac{-2T_3^l}{4\pi\alpha} c_l \sum_k \text{Im}(q_{k2}) \lambda_{kH^+H^-} \left[2 - \frac{2}{h_k} + \frac{2 \ln h_k}{h_k} - \frac{2 - 2h_k + w_k}{h_k - w_k} \ln \frac{h_k}{w_k} \right. \\ \left. - \frac{1 + h_k^2 - h_k(2 + w_k)}{w_k(h_k - w_k)} \ln h_k \ln \frac{h_k}{w_k} - \frac{2(h_k - 2h_k^2 + h_k^3 + w_k - 2h_k w_k)}{h_k^2 w_k} \text{Li}_2 \left(1 - \frac{1}{h_k} \right) \right. \\ \left. + \frac{w_k(1 - 4h_k + 2h_k^2)}{h_k^2(h_k - w_k)} \Phi(h_k) - \frac{1 - h_k^3 - w_k + h_k^2(3 + 2w_k) - h_k(3 + w_k + w_k^2)}{w_k(h_k - w_k)} \Phi(h_k, w_k) \right]. \quad (4.13)$$

Gauge Boson Loop contributions

The Barr-Zee diagrams involving W bosons in the loop are the largest subset of diagrams that contribute to the eEDM. The contributing diagrams are shown in Fig. 4.3. The electromagnetic and neutral Barr-Zee contributions are given by the gauge-dependent expressions as follows

$$\delta_W^{\text{EM}}(\xi) = \delta_W^{\text{EM}} + Q_{\text{EM}}^l c_l \sum_k \text{Im}(q_{k2}) q_{k1} [2 \ln \xi + F_\xi(w_k)] \quad (4.14)$$

and

$$\delta_W^{\text{NC}}(\xi) = \delta_W^{\text{NC}} + \frac{Q_W^l}{4 \sin^2 \theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} [\xi(1 - 2 \sin^2 \theta_W) \Phi(\xi \cos^2 \theta_W) + F_\xi(w_k)]. \quad (4.15)$$

Here, δ_W^i ($i \in [\text{EM}, \text{NC}]$) denote the gauge-independent terms of each contribution. They read

$$\delta_W^{\text{EM}} = Q_{\text{EM}}^l c_l \sum_k \text{Im}(q_{k2}) q_{k1} [4(1 + 6w_k) + 2(1 + 6w_k) \ln w_k - (3 - 16w_k + 12w_k^2) \Phi(w_k)], \quad (4.16)$$

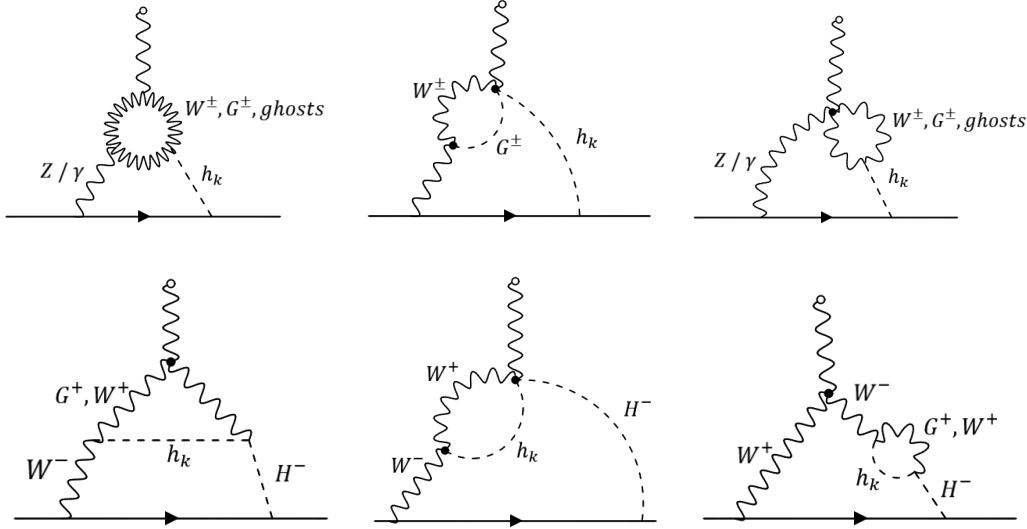


Figure 4.3.: Generic diagrams from contributions with charged W bosons in the loop. The white dot represents the background field $\bar{A}_\mu$. Top row: electromagnetic and neutral current contributions $\delta_W^{\text{EM}}(\xi)$ and $\delta_W^{\text{NC}}(\xi)$. Bottom row: charged current contributions $\delta_W^{\text{CC}}(\xi)$.

and

$$\delta_W^{\text{NC}} = \frac{Q_W^l}{4 \sin^2 \theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} \left[-\frac{3 - 16w_k + 12w_k^2}{1 - z_k} \Phi(w_k) + \frac{1 - 2 \sin^2 \theta_W + 2(5 - 6 \sin^2 \theta_W) w_k}{\cos^2 \theta_W (1 - z_k)} \ln z_k - z_k \frac{1 + 8 \sin^2 \theta_W - 12 \sin^4 \theta_W}{1 - z_k} \Phi(\cos^2 \theta_W) \right]. \quad (4.17)$$

In Eq. (4.14), we introduced a mass-dependent and gauge-dependent function $F_\xi(w_k)$, which reads

$$F_\xi(w_k) = -\xi \ln^2 \xi - 2(1 - \xi)^2 w_k \text{Li}_2(1 - \xi) - [3 + \xi - (1 - \xi)^2 w_k] \ln \xi \ln w_k + \xi(1 - 2\xi w_k) \Phi(\xi w_k) + [3 - \xi - 2(2 - \xi - \xi^2) w_k + (1 - \xi)^3 w_k^2] \Phi(w_k, \xi w_k). \quad (4.18)$$

Now, we consider the charged current Barr-Zee diagrams. The contribution δ_W^{CC} is given by

$$\delta_W^{\text{CC}}(\xi) = \delta_W^{\text{CC}} + \frac{-2T_3^l}{4 \sin^2 \theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} G_\xi(w_k), \quad (4.19)$$

where the gauge-independent term δ_W^{CC} reads

$$\begin{aligned} \delta_W^{\text{CC}} = & \frac{-2T_3^l}{4 \sin^2 \theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} \left[\frac{2}{w_k} - \frac{2(1 - w_k)^2}{h_k w_k} \right. \\ & - \frac{2(1 - w_k) w_k^2 + (2 + w_k) h_k^2 - h_k(2 - w_k - 7w_k^2)}{h_k w_k (h_k - w_k)} \ln w_k + \frac{h_k^2 - 2(1 - w_k)^2 + h_k(1 + 7w_k)}{h_k (h_k - w_k)} \ln h_k \\ & - \frac{(1 - w_k)^3 - 3h_k^2 w_k - h_k(1 + 3w_k - 4w_k^2)}{h_k^2 (h_k - w_k)} \ln \frac{h_k}{w_k} \ln w_k - \frac{2w_k(1 - w_k)^3 + h_k(2 - 8w_k + 6w_k^3)}{h_k^2 w_k^2} \\ & \times \text{Li}_2 \left(1 - \frac{1}{w_k} \right) - \frac{1 - 6w_k + 6w_k^2 + 4w_k^3}{(h_k - w_k) w_k^2} \Phi(w_k) \\ & \left. + \frac{(1 - w_k)^4 - 3h_k^3 w_k - h_k(2 + 5w_k)(1 - w_k)^2 + h_k^2(1 + 7w_k^2)}{h_k^2 (h_k - w_k)} \Phi(h_k, w_k) \right]. \end{aligned} \quad (4.20)$$

Another gauge- and mass-dependent function $G_\xi(w_k)$ has been introduced in Eq. (4.19), which is given by

$$G_\xi(w_k) = -2\xi(1 + \ln \xi) + \left(\frac{(1 - \xi w_k)^2}{w_k^2} - \xi \right) \left[\ln \xi \ln \xi w_k + 2\text{Li}_2 \left(1 - \frac{1}{\xi w_k} \right) \right] \\ - \left[\xi(1 - 3\xi) - \frac{1 - (1 + 3\xi)w_k}{w_k^2} + (1 - \xi)^2 \xi w_k \right] \Phi(w_k, \xi w_k). \quad (4.21)$$

Kite Contributions

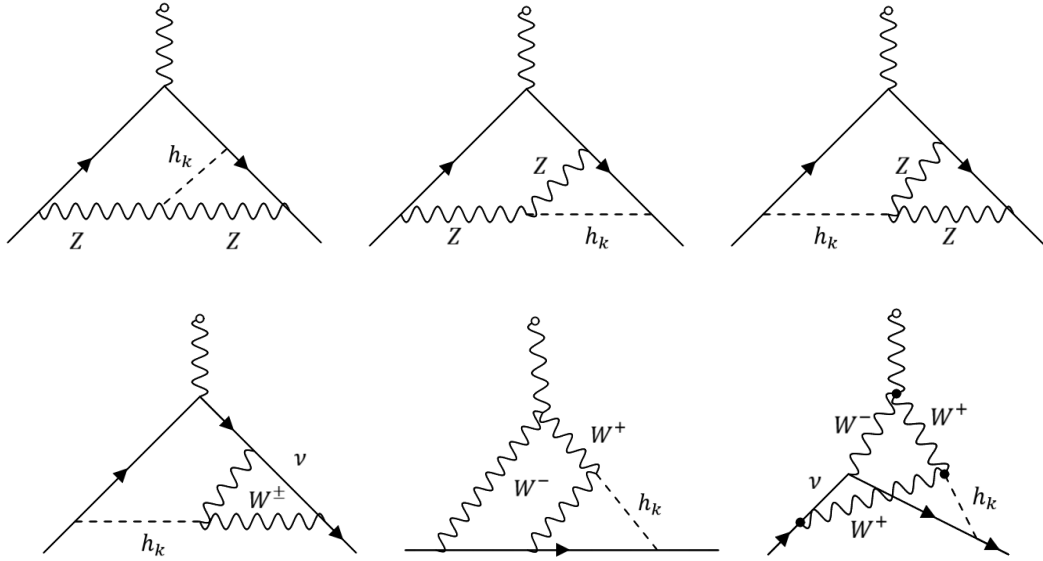


Figure 4.4.: Generic diagrams of the kite class. The white dot represents the background field $\bar{A}_\mu$. Top row: neutral current contributions $\delta_{\text{kite}}^{\text{NC}}$. Bottom row: charged current contributions $\delta_{\text{kite}}^{\text{CC}}(\xi)$.

We will now focus on the bottom half of Tab. 4.1, i.e. the kite diagrams. The neutral-current contributions are gauge-independent. The contribution $\delta_{\text{kite}}^{\text{NC}}$ reads

$$\delta_{\text{kite}}^{\text{NC}} = -Q_{\text{EM}}^l \frac{(Q_W^l)^2 - 1}{8 \sin^2 \theta_W \cos^2 \theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} \frac{1}{z_k^3} \left[z_k^2 + \frac{\pi^2}{6} (1 - 4z_k) - 2z_k^2 \ln(z_k) \right. \\ \left. + \frac{1 - 4z_k}{2} \ln^2(z_k) + 2(1 - 4z_k + z_k^2) \text{Li}_2 \left(1 - \frac{1}{z_k} \right) + \frac{1 - 6z_k + 8z_k^2}{2} \Phi(z_k) \right] \\ - Q_{\text{EM}}^l \frac{(Q_W^l)^2 + 1}{24 \sin^2 \theta_W \cos^2 \theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} \frac{1}{z_k} \left[2z_k(1 - 4z_k) + \frac{\pi^2}{3} (3z_k^2 + 4z_k^3) \right. \\ \left. - 2z_k(1 + 4z_k) \ln(z_k) + 2(1 - 3z_k^2 - 4z_k^3) \text{Li}_2 \left(1 - \frac{1}{z_k} \right) + (1 - 2z_k - 8z_k^2) \Phi(z_k) \right]. \quad (4.22)$$

The complete gauge dependence of the kite diagrams is incorporated in the charged current contribution and is given by

$$\delta_{\text{kite}}^{\text{CC}}(\xi) = \delta_{\text{kite}}^{\text{CC}} + \frac{-2T_3^l}{4 \sin^2 \theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} [F_\xi(w_k) - G_\xi(w_k) + (1 + Q_{\text{EM}}^l) H_\xi(w_k)]. \quad (4.23)$$

Here, a third gauge-dependent function $H_\xi(w_k)$ is introduced; however, this term vanishes after specifying $Q_{\text{EM}}^l = -1$. Therefore, we will not show the analytical formula for this function. The gauge-independent term $\delta_{\text{kite}}^{\text{CC}}$ reads

$$\begin{aligned} \delta_{\text{kite}}^{\text{CC}} = & \frac{-2T_3^l}{4\sin^2\theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} \left[\frac{2\pi^2}{9} w_k (3 + 4w_k) + \frac{2}{3} (5 - 8w_k) - \frac{16}{3} (1 + w_k) \ln w_k \right. \\ & \left. + \frac{2(3 + 2w_k - 6w_k^3 - 8w_k^4)}{3w_k^2} \text{Li}_2 \left(1 - \frac{1}{w_k} \right) + \frac{(1 + 2w_k)(3 - 10w_k + w_k^2)}{3w_k^2} \Phi(w_k) \right]. \end{aligned} \quad (4.24)$$

This concludes the list of eEDM two-loop contributions. In the next section, we will discuss the construction of a gauge-independent eEDM result.

Construction of a Gauge-Independent Result

We obtain the complete eEDM d_e by summing each contribution as

$$\begin{aligned} \frac{d_e}{e} = & \frac{\sqrt{2}G_F m_e}{64\pi^3} \left[\sum_f (\delta_f^{\text{EM}} + \delta_f^{\text{NC}}) + (\delta_{H^+}^{\text{EM}} + \delta_{H^+}^{\text{NC}} + \delta_{H^+}^{\text{CC}}) \right. \\ & \left. + (\delta_W^{\text{EM}}(\xi) + \delta_W^{\text{NC}}(\xi) + \delta_W^{\text{CC}}(\xi) + \delta_{\text{kite}}^{\text{NC}} + \delta_{\text{kite}}^{\text{CC}}(\xi)) \right] \end{aligned} \quad (4.25)$$

The complete gauge dependence of the eEDM is incorporated in the Barr-Zee diagrams with a W boson loop and in the charged-current kite diagrams. By summing only the gauge-dependent terms, we obtain the following relation

$$\begin{aligned} & \left. \delta_W^{\text{EM}}(\xi) + \delta_W^{\text{NC}}(\xi) + \delta_W^{\text{CC}}(\xi) + \delta_{\text{kite}}^{\text{CC}}(\xi) \right|_{\xi\text{-dep.}} = \\ & \frac{1}{4\sin^2\theta_W} c_l \sum_k \text{Im}(q_{k2}) q_{k1} \left[(Q_W^l - 2T_3^l + 4Q_{\text{EM}}^l \sin^2\theta_W) F_\xi(w_k) \right. \\ & \left. - 2T_3^l (1 + Q_{\text{EM}}^l) H_\xi(w_k) + 8Q_{\text{EM}}^l \sin^2\theta_W \ln \xi + Q_W^l (1 - 2\sin^2\theta_W) \Phi(\xi \cos^2\theta_W) \right]. \end{aligned} \quad (4.26)$$

The $G_\xi(w_k)$ terms immediately cancels between the charged current Barr-Zee diagrams $\delta_W^{\text{CC}}(\xi)$ and the kite diagrams $\delta_{\text{kite}}^{\text{CC}}(\xi)$. The $F_\xi(w_k)$ and $H_\xi(w_k)$ contributions vanish after the insertion of the relations $Q_{\text{EM}}^l = -1$ and $Q_W^l = 2T_3^l - 4Q_{\text{EM}}^l \sin^2\theta_W$. The terms without a mass-dependence go to zero after summing over k and using the relation $\sum_k q_{1k} q_{2k} = 0$. Therefore, all gauge-dependent terms vanish, such that we obtain the final result of the two-loop eEDM, which reads

$$\begin{aligned} \frac{d_e}{e} = & \frac{\sqrt{2}\alpha(\mu)G_F m_e}{64\pi^3} \left[\sum_f (\delta_f^{\text{EM}} + \delta_f^{\text{NC}}) + (\delta_{H^+}^{\text{EM}} + \delta_{H^+}^{\text{NC}} + \delta_{H^+}^{\text{CC}}) \right. \\ & \left. + (\delta_W^{\text{EM}} + \delta_W^{\text{NC}} + \delta_W^{\text{CC}} + \delta_{\text{kite}}^{\text{NC}} + \delta_{\text{kite}}^{\text{CC}}) \right]. \end{aligned} \quad (4.27)$$

Note that only the sum of these contributions is gauge-independent.¹⁰ The individual contributions are still gauge-dependent. Note that, in recent work, the one-loop contributions were also considered; however, in our analysis, we found that these contributions are always below the experimental limits. Therefore, we omitted these contributions in our analysis.

¹⁰We verified this explicitly.

Fermion Masses used in the EDM Calculation

An additional question, aside from which diagrams to include, arises regarding the choice of the renormalization scheme. Explicitly, two different schemes can be employed regarding the fermion mass renormalization. The most common renormalization schemes used for the top and bottom masses are the $\overline{\text{MS}}$ masses evaluated at the scale $\mu = M_Z$ ($\overline{m}_t(M_Z), \overline{m}_b(M_Z)$) [41, 78, 80] or the pole mass used for the top quark and the running $\overline{\text{MS}}$ bottom quark mass evaluated at the scale $\mu = \overline{m}_b$, i.e., $(m_t, \overline{m}_b(\overline{m}_b))$ [39, 81–83]. For the third generation lepton τ , we always use the pole mass m_τ . For brevity, we will refer to the first choice as M_Z -masses scheme and to the second choice as "pole masses" scheme. In previous work [84], that did not include the full two-loop calculation including the kite contribution in the eEDM, it has been shown that the choice of the used renormalization scheme has an impact on the phenomenological results. Here, in the Type-II of the C2HDM, with $h_2 = h_{125}$ has been investigated. By evaluating the fermions at the M_Z scale, it has been found that a sizeable CP-odd component in $h_{\text{SM}} b \bar{b}$ is excluded by the combined experimental constraints from the upper limit on the eEDM and from the cross-section limits searches for BSM scalars. On the other hand, by using the pole mass scheme, the possibility of sizeable CP-odd components remained possible. We will investigate these statements in this work in light of the updated eEDM calculation with the additional kite contributions.

Numerical Setup of the Analysis

The goal of our analysis is to probe the CP nature of the SM-like Higgs boson. To achieve this, we perform an extensive scan of the parameter space, constrained by all relevant theoretical and experimental constraints. In the next section, we will briefly present all experimental and theoretical constraints used in our analysis.

5.1. Experimental and Theoretical Constraints

5.1.1. Theoretical Constraints

In principle, one can choose the input parameters given in Eq. (2.61) freely. However, not every combination of parameters will constitute a valid parameter point, as these parameters must still satisfy theoretical and experimental constraints. To obtain a point, which is consistent by theory, it has to fulfill the condition that the potential is bounded from below and has a global minimum with a VEV of $v = 246$ GeV, such that the physics described in this model is stable and consistent with phenomenology. Furthermore, the chosen input parameters must satisfy the condition of perturbative unitarity. In the next two subsections, we discuss the conditions associated with these constraints to ensure that the parameter points are theoretically consistent. In our analysis, these conditions are implemented and checked for each parameter point.

Boundedness from Below and Global Minimum

To obtain a global minimum, the potential needs to be bounded from below. To ensure this condition, the potential parameters need to fulfill the following conditions [85, 86]

$$0 < \lambda_1 \tag{5.1a}$$

$$0 < \lambda_2 \tag{5.1b}$$

$$-\sqrt{\lambda_1 \lambda_2} < \lambda_3 + \min(0, \lambda_4 - |\lambda_5|) . \tag{5.1c}$$

In the C2HDM, it is in principle possible to obtain charge- or CP-breaking extrema, in addition to the CP-conserving extrema. In previous works [87–92], however, it has been shown that if a CP-conserving solution exists, it will always correspond to the minimum of

the potential. In that case, the CP-odd and charge-breaking solutions are saddle points. It has been shown [93] that the condition for the C2HDM to obtain a global minimum is given by

$$\left[\left(\frac{m_{H^\pm}^2}{v^2} + \frac{\lambda_4}{2} \right)^2 - \frac{|\lambda_5|^2}{4} \right] \left[\frac{m_{H^\pm}^2}{v^2} + \frac{\sqrt{\lambda_1 \lambda_2} - \lambda_3}{2} \right] > 0. \quad (5.2)$$

Perturbative Unitarity

We require that perturbative unitarity be satisfied at the tree level. This condition is fulfilled if the S -matrix is unitary. This is obtained if the eigenvalues of the $2 \rightarrow 2$ scattering matrix are smaller than 8π . The eigenvalues κ_i ($i \in [1, \dots, 9]$) have been evaluated in [94–96] and are given by

$$\kappa_{1,\pm} = \frac{3}{2}(\lambda_1 + \lambda_2) \pm \sqrt{\frac{9}{4}(\lambda_1 - \lambda_2) + (2\lambda_3 + \lambda_4)^2}, \quad (5.3a)$$

$$\kappa_{2,\pm} = \frac{1}{2}(\lambda_1 + \lambda_2) \pm \frac{1}{2}\sqrt{(\lambda_1 - \lambda_2)^2 + 4\lambda_4^2}, \quad (5.3b)$$

$$\kappa_{3,\pm} = \frac{1}{2}(\lambda_1 + \lambda_2) \pm \frac{1}{2}\sqrt{(\lambda_1 - \lambda_2)^2 + 4|\lambda_5|^2}, \quad (5.3c)$$

$$\kappa_4 = \lambda_3 + 2\lambda_4 - 3|\lambda_5|, \quad (5.3d)$$

$$\kappa_5 = \lambda_3 - |\lambda_5|, \quad (5.3e)$$

$$\kappa_6 = \lambda_3 + 2\lambda_4 + 3|\lambda_5|, \quad (5.3f)$$

$$\kappa_7 = \lambda_3 + |\lambda_5|, \quad (5.3g)$$

$$\kappa_8 = \lambda_3 + \lambda_4, \quad (5.3h)$$

$$\kappa_9 = \lambda_3 - \lambda_4. \quad (5.3i)$$

We then check the following conditions, to ensure that the parameter point is valid under this constraint

$$\max(|\kappa_i|) \leq 8\pi. \quad (5.4)$$

5.2. Experimental Constraints

Electroweak Precision Measurements

Measurements of electroweak observables are sensitive to loop-induced effects from new physics. If the BSM effects are captured completely by the self-energy corrections to the gauge boson propagators, one can parametrize these effects through the oblique parameters S , T , and U [97, 98]. To obtain a valid parameter point, we require that these agree at the 2σ level with the global fit of Ref. [99], which is given by

$$S = 0.04 \pm 0.11, \quad T = 0.09 \pm 0.14, \quad U = 0.02 \pm 0.11. \quad (5.5)$$

Flavour Constraints

From the rare B -meson decays, in particular the process $b \rightarrow s\gamma$, we obtain constraints for the charged scalar mass $m_{H^\pm}$. We incorporate this constraint using the formula from Ref. [100]. Here, we require that the result agrees with the experimental measurement at 3σ [101]. It has been shown [102–106] that this implies a lower bound of $m_{H^\pm} \geq 580$ GeV at 95% CL for the Type II C2HDM. Additionally, the global fit of Ref. [99] confirms this lower bound and also shows that this also holds for the Lepton flipped type.

Higgs Data

Higgs measurements at the LHC further constrain the parameter space. We check that the signal strengths μ_{VBF}^{ff} ($ff \in [WW, \gamma\gamma, \tau\tau, bb, ZZ]$), which are given by

$$\mu_{\text{VBF}}^{ff} = \frac{\sigma(pp \rightarrow h_{125})_{\text{2HDM}} \text{BR}(h_{125} \rightarrow ff)_{\text{2HDM}}}{\sigma(pp \rightarrow h_{125})_{\text{SM}} \text{BR}(h_{125} \rightarrow ff)_{\text{SM}}} \quad (5.6)$$

are consistent with the data obtained from the ATLAS collaboration [107] at 2σ . Further, we impose that the coupling modifiers are in agreement with the ATLAS measurements [108] at 3σ .

Direct searches for additional scalars are accounted for using the public code `HiggsTools` [109] and the `HiggsBounds` module [110].

Measurement of the CP Properties of the SM-like Higgs boson

After applying the Higgs constraints, we apply the constraints on the CP properties of the SM-like Higgs boson from LHC direct searches. Here, we demand that the CP-violating couplings of $h_{\text{SM}} t \bar{t}$ fulfills the following relation [111]

$$|\theta_t| = \left| \arctan \frac{c_t^o}{c_t^e} \right| < 43^\circ \text{ at } 95\% \text{ CL} . \quad (5.7)$$

For the CP-odd couplings of $h_{\text{SM}} \tau \bar{\tau}$, we are investigating two different approaches. In the first approach, we use the module `HiggsSignals` [112] within `HiggsTools`, which uses a likelihood estimate. The second approach is to apply the following upper limit to θ_τ [113, 114]

$$|\theta_\tau| = \left| \arctan \frac{c_\tau^o}{c_\tau^e} \right| < 34^\circ \text{ at } 95\% \text{ CL} . \quad (5.8)$$

Electron Electric Dipole Moment

We further impose that our parameter points comply with the measurement of JILA [71] given by

$$|d_e| < 4.10 \times 10^{-30} \text{ e.cm} . \quad (5.9)$$

Therefore, we calculate, for each parameter point, the eEDM using Eq. (4.27) and compare it with the experimental data.

5.3. Scan Ranges

In our analysis, we are mainly interested in the Type II C2HDM. In our analysis, we consider the case $m_2 = m_{125}$, where $m_{125} = 125.09 \text{ GeV}$. Further, we use the following SM input values

$$\begin{aligned} G_F &= 1.16638 \times 10^{-5} \text{ GeV}^{-2} & M_Z &= 91.1876 \text{ GeV} \\ \alpha_{\text{em}}^{-1}(M_Z) &= 127.92 & M_W &= 80.385 \text{ GeV} \\ \alpha_{\text{em}}^{-1} &= 137.035999 & m_\tau &= 1.77682 \text{ GeV} \\ m_t &= 172.5 \text{ GeV} & \bar{m}_t(M_Z) &= 163 \text{ GeV} \\ \bar{m}_b(\bar{m}_b) &= 4.78 \text{ GeV} & \bar{m}_b(M_Z) &= 2.88 \text{ GeV} \\ \Gamma_W &= 2.08430 \text{ GeV} & \Gamma_Z &= 2.49427 \text{ GeV} . \end{aligned} \quad (5.10)$$

Parameter	Range	
	Lower	Upper
m_1	30 GeV	1000 GeV
m_2	125.09	125.09 GeV
v_S	1 GeV	1000 GeV
$\tan\beta$	0.3	30
$\text{Re}(m_{12})$	$\pm 10^{-1}$	$\pm 10^7$
$\alpha_1, \alpha_2, \alpha_3$	$-\frac{\pi}{2}$	$\frac{\pi}{2}$

Table 5.1.: Parameter ranges used in the scan.

In Tab. 5.1, the parameter ranges of our scan are summarized. As the third mass m_3 is a derived quantity, it can become negative. These points are discarded as they are not physical.

We employ two different scan strategies, which we label Strategy 1 and Strategy 2. The approach adopted in Strategy 1 is a guided scan. Here, we explore the parameter space near the phenomenological boundaries and iteratively increase the CP-odd component of the $h_{\text{SM}} f \bar{f}$ coupling. This approach has also been used in Refs. [115]. By incrementally adjusting the coupling strength, we can map out the allowed parameter space while maintaining control over theoretical and experimental constraints. Strategy 2 consists of an AI-based black-box optimization technique. We will discuss the algorithms used in Strategy 2 in more detail in Ch. 7. In the following chapters, we will present the results of our numerical analysis for both strategies. We will begin our discussion with Strategy 1.

Phenomenology with Strategy 1

In the following chapter, we will present the results obtained with Strategy 1 in the Type-II C2HDM, with $h_2 = h_{125}$. The approach adopted in Strategy 1 is a guided scan, wherein we explore the parameter space near the phenomenological boundaries. Specifically, we iteratively increase the CP-odd component of the $h_{\text{SM}} f \bar{f}$ coupling, allowing for a systematic investigation of its effects. By incrementally adjusting the coupling strength, we map out the allowed parameter space while ensuring alignment with both theoretical predictions and experimental constraints. In the calculation of the eEDM, we included the usual Barr-Zee diagrams and additionally the contributions of the kite diagram, which we described in Sec. 4.1. Here, we use the MZ mass scheme to renormalize the fermion masses. Note that we consider only third-generation fermions in the corresponding Barr-Zee diagrams in this chapter. All parameter points were additionally confirmed via the public code **ScannerS** [96, 116], which has been updated in the scope of this work to include the kite contributions in the EDM calculation.

6.1. Results

In Fig. 6.1, we show the CP-odd coupling of the Higgs boson to a bottom quark pair $\text{sign}(k_V)c_b^o$ (cf. Eq. (2.68)) as a function of CP-even coupling of the Higgs boson to a bottom quark pair $\text{sign}(k_V)c_b^e$ (cf. Eq. (2.67)). On the left, we imposed the current EDM limit given in Eq. (5.9). On the right, we plot the expected limit of $1.0 \times 10^{-33} \text{e.cm}$. The red points fulfill all constraints given in the previous chapter, except the ones on θ_τ . The blue points satisfy all constraints, including the limit on θ_τ given in Eq. (5.8). The purple points, instead, satisfy all constraints when the θ_τ constraint is imposed via **HiggsSignals**. This figure shows that the valid points cluster around the SM solution, i.e., $(\text{sign}(k_V)c_b^o, \text{sign}(k_V)c_b^e) = (0, 1)$. Furthermore, in our scans with Strategy 1, it can be seen that no valid points around the "wrong-sign" solution [117, 118], i.e., $(\text{sign}(k_V)c_b^o, \text{sign}(k_V)c_b^e) = (0, -1)$ can be found. Note that parameter points with sizable CP-odd couplings can still be obtained, even under more stringent eEDM bounds [72–74], as shown in the right plot of Fig. 6.1.

Next, we want to investigate the impact of the kite diagrams on the parameter space. Figure 6.2 shows the electron EDM as a function of the mixing angle α_2 . As above, the left plot fulfills the current EDM limit, while the right plot is more constrained by the projected EDM

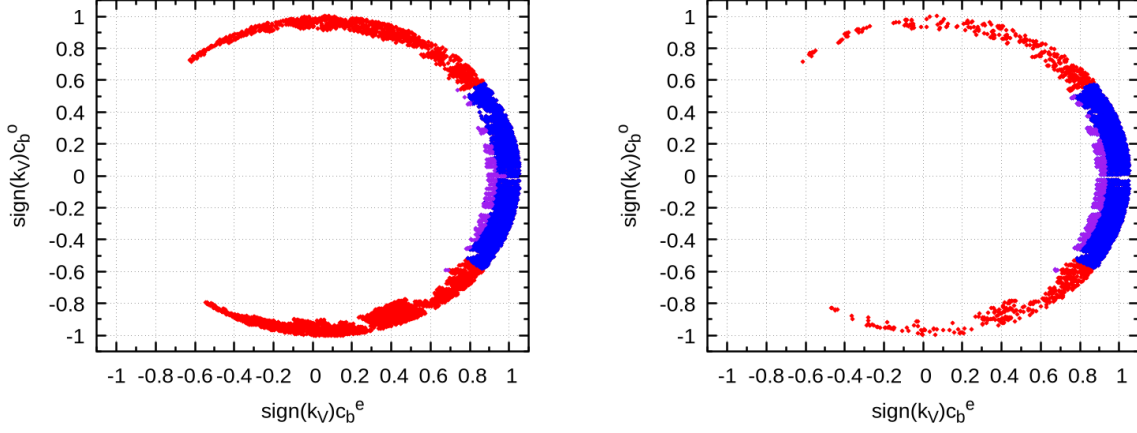


Figure 6.1.: $\text{sign}(k_V)c_b^o$ as a function of $\text{sign}(k_V)c_b^e$ using Strategy 1 in the Type-II C2HDM with $h_{125} = h_2$. Red points: all constraints included except those related to θ_τ . Purple (blue) points: All constraints included and constraints on θ_τ implemented via `HiggsSignals` (Eq. (5.8)). Left panel: current eEDM limit $4.1 \times 10^{-30} \text{ e} \cdot \text{cm}$. Right panel: projected eEDM limit $1.0 \times 10^{-33} \text{ e} \cdot \text{cm}$. Figure has been published in [40].

limit. The green points show the dominant EDM contribution; the red points show only the EDM contributions from the Barr-Zee diagrams. The blue points show the predicted total EDM, including the contributions from the kite diagrams (cf. Eq. (4.27)), which is the gauge-boson loop contribution. This plot confirms the results of Ref. [41], that the kite diagrams can be of the same order as the Barr-Zee diagrams. Further, Fig. 6.2 shows that there are large cancellations between the EDM contributions.

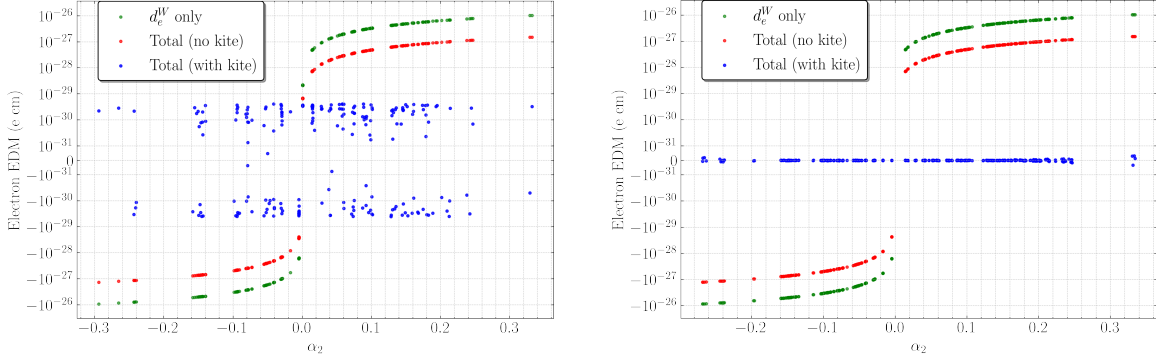


Figure 6.2.: Electron electric dipole moment as a function of the mixing angle α_2 . Green points denote the dominant contribution channel. Red (blue) points show the total eEDM without (with) kite contribution. Left panel: current eEDM limit $4.1 \times 10^{-30} \text{ e} \cdot \text{cm}$. Right panel: projected eEDM limit $1.0 \times 10^{-33} \text{ e} \cdot \text{cm}$. The figure has been published in Ref. [40].

Phenomenology with Machine Learning Algorithms

In the previous chapter, we used a guided-scan method to obtain the parameters. However, Ref. [119] shows that when using machine learning (ML) algorithms to scan the parameter space, the traditional method often misses a large portion of the valid parameter space, with significant consequences for phenomenological interpretations. This motivated us to use these ML algorithms within the C2HDM framework. In general, ML has become essential for particle physics analysis [120–124]. In particular, it has become essential for data analysis in experiments like the LHC, as the data obtained has become more complex and the sample sizes have grown larger. We are interested in exploring the parameter space of BSM theories. Given the goal of discovering the unknown physical implications in a highly constrained parameter space, we employ scan techniques that do not rely on an initial set of sampled data. We use the CMA-ES algorithm first developed in Ref. [125], with an additional histogram-based anomaly-detection component used for the Novelty Reward [126]. This approach allows us to explore the parameter space and the physical observables in our model. Figure 7.1 shows a sketch of an approach to obtain valid parameter points with ML techniques. We first initialize a multivariate normal distribution with a randomly chosen mean value, and the corresponding covariance matrix is equal to the unity matrix multiplied by a global factor σ . From this distribution, parameter points are sampled, which are then checked with a Fortran code and validated by **ScannerS** for the relevant experimental and theoretical constraints. We have shown these in Sec. 5.1. Next, we introduce for each individual constrained quantity $\mathcal{O}$, a function $\mathcal{C}(\mathcal{O})$ which reads

$$\mathcal{C}(\mathcal{O}) = \max(0, -\mathcal{O} + \mathcal{O}_{\text{LB}}, \mathcal{O} - \mathcal{O}_{\text{UB}}). \quad (7.1)$$

Here, we introduced $\mathcal{O}_{\text{LB}}$ and $\mathcal{O}_{\text{UB}}$ that denote the lower and upper limit of the constrained quantity. Equation (7.1) is zero if $\mathcal{O}$ lies in the specified interval. Otherwise, it returns a positive number indicating how far it is from the bound. As we have multiple constraints, we define a single loss function L , which reads

$$L = \sum_i^{N_c} \mathcal{C}(\mathcal{O}_i), \quad (7.2)$$

where N_c is the number of constrained quantities. As depicted in Fig. 7.1, we use the Covariant Matrix Adaption Evolutionary Strategy (CMA-ES) to minimize Eq. (7.2), by iteratively

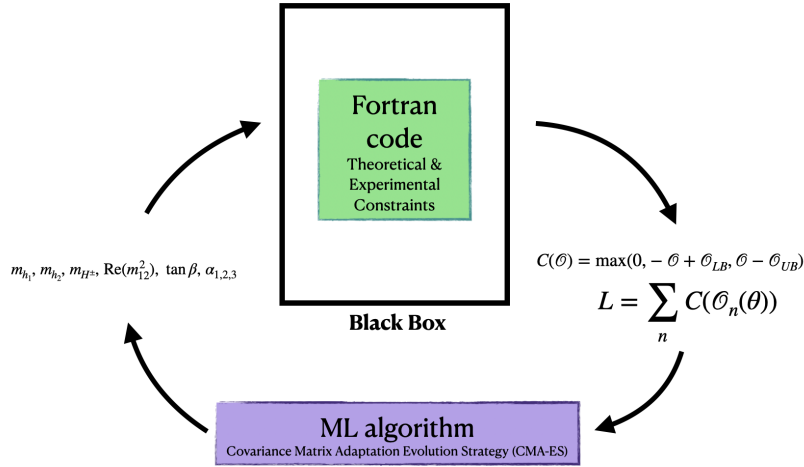


Figure 7.1.: Flowchart of the used Workflow.

optimizing the initial distribution. In the following section, we will further describe this strategy.

7.1. Covariant Matrix Adaptation Evolutionary Strategy

Evolutionary strategies (ES) use an iterative process in which possible solutions to a given problem are tested, and the best are used to generate new ones. In BSM physics, the solution to the problem is to find valid parameter points that minimize Eq. (7.2). In contrast to Genetic Algorithms, ES does not use a previously sampled data set to generate new points. Instead, the new solutions are generated from a distribution called the generation. The points for each generation are sampled from the parameter distributions based on the best candidates from the previous iteration. In CMA-ES, the distribution is a multivariate normal distribution $\mathcal{N}^i(m_i, C_i)$, where m_i denotes the mean value and C_i is the covariance matrix of the i -th generation. As stated before, we initialize the normal distribution with a random point as its mean, and set the covariance matrix to the identity matrix multiplied by a global factor σ . From this distribution, λ candidates are generated, and their suitability is checked with Eq. (7.2). Afterwards, the best μ candidates are sorted and from these a new distribution $\mathcal{N}^{i+1}(m_{i+1}, C_{i+1})$ are generated, with a new mean m_{i+1} and a new covariant matrix C_{i+1} . This procedure is expected to behave similarly to first- and second-order optimization methods. The mean is updated along the direction of steepest descent of the loss function, while the covariance matrix provides an approximation to its Hessian. However, CMA-ES does not calculate the derivatives of the loss function, which in fact means that one can use it on nonconvex, ill-conditioned, and non-continuous loss functions. This has the advantage that the algorithm converges quickly and can be applied to various applications. For further information on this strategy, we refer to Ref [125].

7.2. Histogram Based Outlier System

A major advantage of CMA-ES is the quick convergence compared to other black-box search algorithms. The caveat of this algorithm is that the explored parameter space is highly localized. In our approach, which was also applied in Ref. [126], we add a novelty reward to the loss function. Here, we calculate the point density and add it to the loss function as

a penalty to improve the exploration of the parameter space. This ensures that when the loss function is minimal, new valid points are found, while also avoiding parameter regions that have already been explored. The additional penalty to the loss function could lead to new local minima, spoiling the exploration of valid parameter points. To circumvent this problem, we add an additional factor of one outside the valid region. For this we consider a new function $\tilde{L}$, which reads

$$\tilde{L} = \begin{cases} 1 + L, & \text{if } L > 0 \\ 0, & \text{if } L = 0 \end{cases} . \quad (7.3)$$

With Eq. (7.3), it is possible to calculate the total loss function L_T , which is given by

$$L_T = \tilde{L} + \frac{1}{N_p} \sum_{i=1}^{N_p} p_i , \quad (7.4)$$

where N_p are the number of penalties and p_i is the i -th penalty. With this new loss function, we find a valid point when

$$L = \sum_i^{N_c} \mathcal{C}(\mathcal{O}_i) \Leftrightarrow 0 \leq L_T \leq 1 , \quad (7.5)$$

and invalid points if $L_T \geq 1$. In our case, the point density describes our penalty. For this, we need to compute this quantity. In the literature, this problem is known as density estimation [127], which can be very difficult to address in multidimensional problems such as those in particle physics. In our analysis, we used the Histogram Based Outlier System (HBOS). This algorithm constructs for each parameter θ_j of the point θ a histogram with a fixed number of bins N_{bins} . The penalty for the point θ is then given by summing the individual heights h_j of the bins of the parameter θ_j . Further, a normalization is done such that the penalty $p_j \in [0, 1]$. Therefore, a new parameter point has a penalty of zero, while a point similar to already obtained points has a penalty of one. We note that it is also possible to penalize only a subset of the parameters, allowing us to focus on the exploration of specific model parameters. Furthermore, we can penalize not only the model parameters but also physical quantities, such as the CP-odd angle given in Eq. (5.8). This allows us to explore not only the valid parameter space but also to find new phenomenological characteristics of the BSM theory.

7.3. Phenomenology with Strategy 2

As discussed earlier, scans performed with Strategy 1 often miss a portion of the parameter space, even though they are valid. In chapter 6, we discussed the findings of the plane $\text{sign}(k_V)c_b^o$ vs. $\text{sign}(k_V)c_b^e$ using Strategy 1. In this section, we will redo the analysis, however, now using Strategy 2. Here, we use the ML techniques described in the previous section. We designed the simulations such that they can determine the maximal allowed CP-odd coupling, while still complying with the constraints from θ_τ , implemented either with `HiggsSignals` or via Eq. (5.8). To ensure the exploration of the parameter space, we implemented the novelty reward mechanism, described in Sec. 7.2, on large CP-odd fermion couplings. As in Strategy 1, we included both the kite and Barr-Zee contributions in the EDM calculation.

MZ-Masses Scheme vs. Pole-Masses Scheme

Figure 7.2 shows the plane $\text{sign}(k_V)c_b^o$ vs. $\text{sign}(k_V)c_b^e$. Here, the EDM calculation has been performed in the MZ masses scheme (pole masses scheme) on the left (right) plot. The red points fulfill all constraints given in Sec. 5.1 except the ones on θ_τ . The purple (blue)

points fulfill all constraints, including the ones from θ_τ , where these have been checked via **HiggsSignals** (via Eq. (5.8)). Comparing Figs. 7.2 and 6.1, one can observe important differences. Using the ML algorithm, it is possible to find a larger, previously overlooked valid parameter space when using Strategy 1 to explore the parameter region. This, in particular, shows the strength of ML in these kinds of searches. Also, Fig. 7.2 shows that in both renormalization schemes for the fermion masses, the results are qualitatively similar. We have tested that once we exclude the kite diagrams from the calculation, this similarity no longer exists. This confirms the findings given in Ref. [84]. This, again, shows the importance of considering the kite diagrams in the eEDM calculation. As a phenomenological consequence, sizable CP-odd coupling values $|c_b^o|$ are viable in the C2HDM Type-II with $h_2 \equiv h_{125}$. The parameter space is mainly constrained by the limit of θ_τ . This is evident from the color coding of the points. The blue points cover the same width as the red points in the ellipse, but are truncated at the $|\theta_\tau| \geq 34^\circ$ due to the constraint of Eq. (5.8). On the other hand, the purple points have a thinner width than the red points, but are not constrained by the upper limit of Eq. (5.8). These patterns are features of the likelihood estimation given by **HiggsSignals**.

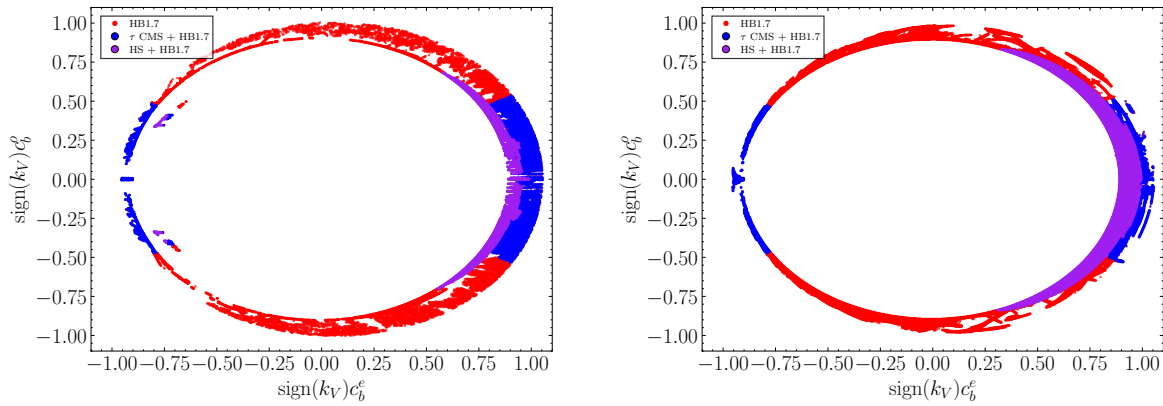


Figure 7.2.: $\text{sign}(k_V)c_b^o$ as a function of $\text{sign}(k_V)c_b^e$ using Strategy 2 in the Type-II C2HDM with $h_{125} = h_2$. Blue points: all constraints included except those related to θ_τ . Purple (blue) points: All constraints included and constraints on θ_τ implemented via **HiggsSignals** (Eq. (5.8)). Left: eEDM calculated in the M_Z -masses scheme. Right: eEDM calculated in the pole-masses scheme. The figure has been published in [40].

Charm quark contribution

In the figures shown previously, we considered only parameter points for which the EDM was calculated using third-generation fermions. Due to the increasingly stringent bounds on the EDM measurement, one could argue that the inclusion of the charm quark¹¹ contributions could become relevant. Indeed, we will show that these contributions become relevant. To prove this point, we recalculated the EDMs of some of the points shown in the left panel of Fig. 7.2, now including the charm-quark contribution. For this calculation, we choose the $\overline{MS}$ charm quark mass evaluated at $\overline{m}_c$, i.e., $\overline{m}_c(\overline{m}_c) = 1.2$ GeV. In Figure 7.3, we show the EDM as a function of the mixing angle α_2 . The green points indicate the dominant contribution, which stems from the gauge boson contributions, the pink points denote the kite contribution, and the green points are the fermionic Barr-Zee contributions, where we inserted only the charm quark mass. As can be seen, the charm quark contributions are of order 10^{-29} e.cm,

¹¹We also considered the case where we include strange quarks; however, these contributions are always several orders of magnitude below the experimental measurements due to their mass suppression. Therefore, we omitted these contributions in our calculation.

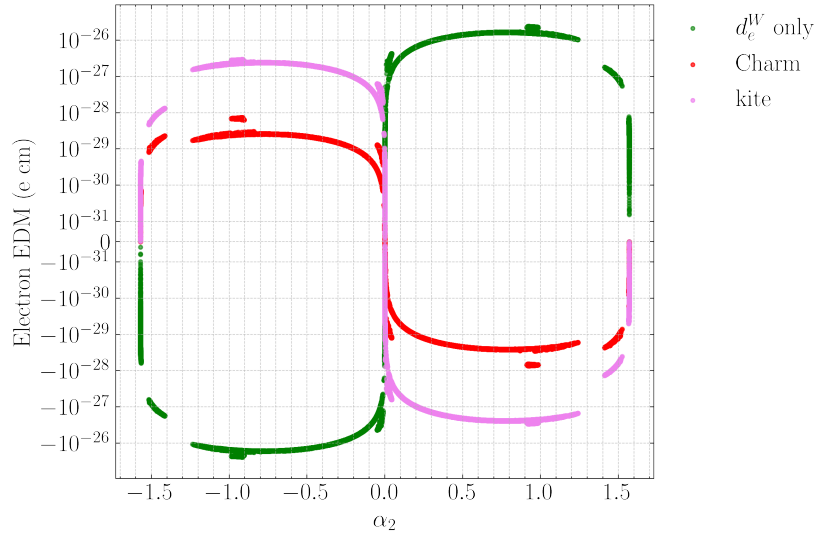


Figure 7.3.: eEDM as a function of the mixing angle α_2 , where the M_Z scheme was used. Green points denote the dominant contribution, the pink points show the kite contribution, and the red points denote the charm quark contribution. Taken from Ref. [40].

which is above the experimental limit. Therefore, points that were previously valid are no longer valid once the charm contributions are included, as this inclusion spoils the delicate cancellations required in the EDM calculation. Nonetheless, even though previously valid points are found to be invalid, it is still possible to find new points where the cancellations, including the charm quark contribution, occur. In Fig. 7.4, we present $\text{sign}(k_V)c_b^o$ as a function of $\text{sign}(k_V)c_b^e$. The color coding of the points corresponds to that of Fig. 7.2. The difference compared to Fig. 7.2, is that we now used the charm quark contribution in the eEDM calculation. Comparing both plots shows that there is no qualitative change in the phenomenology of c_b^o .

Analysis on other Types of the C2HDM

In the previous sections, we established the importance of including the kite contribution in the calculation and also how the ML algorithm can significantly improve the phenomenological analysis. Now, we want to explore other types of the C2HDM. We start with Type I. As the pseudoscalar coupling of all fermions is universal, that particular Type is strongly constrained by the measurement of the top-quark sector. These constraints force the coupling to be close to the SM value for all mass orderings. We also confirmed the statement of Ref. [84], that there are no valid parameter regions with large $|c_b^o|$ for Type II and Flipped models with $h_{1,3} = h_{125}$. In Fig. 7.5, we present our results for the Flipped model with $h_2 = h_{125}$. The color coding is similar to Fig. 7.2. In this calculation, we considered both the kite diagrams and the charm quark contributions in our analysis. In the Flipped model with $h_2 = h_{125}$, we find that it is possible to obtain maximal $|c_b^o|$ couplings, i.e., $|c_b^o| = 1$, which complies with all experimental data. This means that the SM-like Higgs boson couples as a pure pseudoscalar to the bottom quark, whereas it couples as a pure scalar to the top quarks.

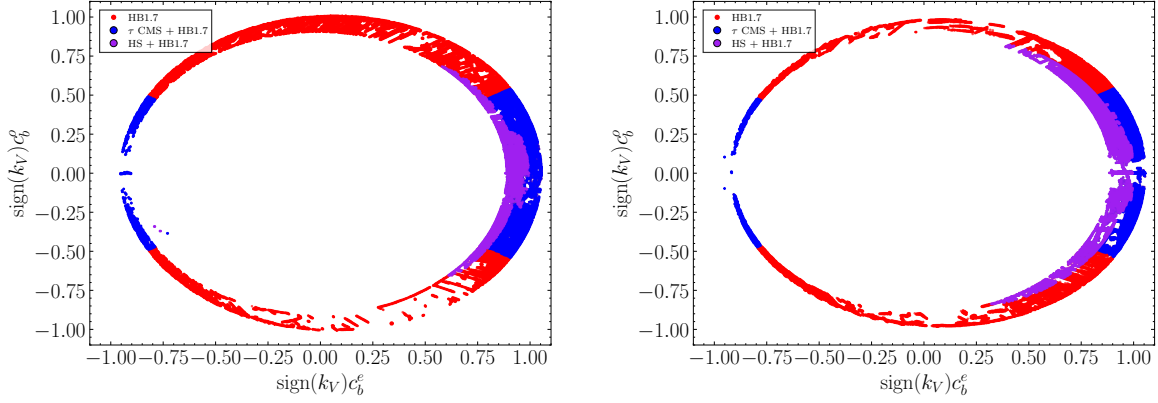


Figure 7.4.: Same Figure as in Fig. 7.2. Here, we additionally included the charm contributions in the eEDM calculation. Taken from Ref. [40].

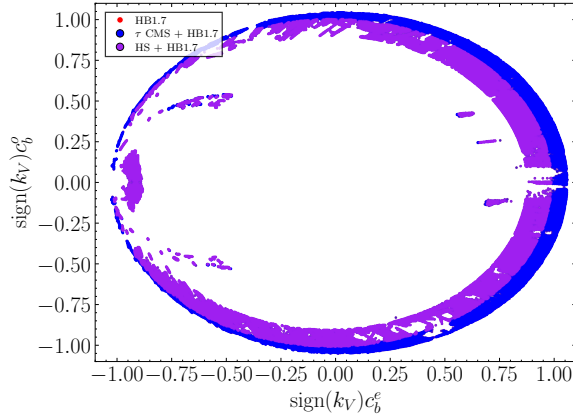


Figure 7.5.: $\text{sign}(k_V)c_b^o$ as a function of $\text{sign}(k_V)c_b^e$ using Strategy 2 in the Flipped type of the C2HDM with $h_{125} = h_2$. The same color coding is used as in Fig. 7.2. Note that the red points lie beneath all the other points. Taken from [40].

In this part of the thesis, we investigated the impact of the collider and eEDM constraints on the parameter space of the C2HDM, which we introduced in Sec. 2.3.

We first introduced the formulas used for the full two-loop eEDM calculation, including a new class of diagrams, the so-called kite diagrams. Furthermore, we investigated the dependence on the renormalization scheme used for the fermion masses in the eEDM calculation. Afterwards, we gave an overview of the theoretical and experimental constraints applied in our study. In the case of constraints arising from measurements of the CP properties of the SM-like Higgs boson, we distinguished how to apply these constraints. Here, we studied the impact of applying the constraints on the CP-violating coupling of $H_{\text{SM}}\tau\bar{\tau}$, either with the public tool `HiggsTools` or with Eq. (5.8).

In Chapter 6, we then performed a guided parameter scan, which we dubbed Strategy 1, for the Type II C2HDM with $h_2 = h_{125}$. We have shown that with this scan method, one obtains valid parameter points that scatter around the SM-like solution. Furthermore, we investigated the impact of the kite diagrams on the parameter space. Here, we have confirmed that the kite diagrams are of the same order as the Barr-Zee diagrams, and therefore need to be included in the analysis of the eEDM.

In Chapter 7, we introduced the ML algorithms we used in our second scan method, dubbed Strategy 2. Here, we used the CMA-ES algorithm with an additional anomaly-detection component as a novelty reward. Using these ML algorithms, we then performed an extensive parameter scan. First, we analyzed the impact of the renormalization scheme choice for the fermion masses. We saw that with the inclusion of the kite diagrams, one obtains qualitatively the same results. This is in contrast to the previously obtained results in Ref. [84], where the kite diagrams were not included in the eEDM calculation. In addition, we showed that using ML algorithms can reveal previously overlooked valid parameter regions. Next, we discussed the impact of including the charm quark in the eEDM calculation. Here, we saw that the charm quark contribution to the eEDM is of order 10^{-29}e.cm , which is larger than the experimental limits. Therefore, including this contribution is necessary to obtain a correct estimate of the eEDM in the C2HDM. It does not change qualitatively the phenomenology on the CP-odd coupling c_b^o , however. Lastly, we briefly commented on the other cases of the C2HDM and provided an update on the possibility of sizeable CP-odd couplings in other types of the model.

In summary, we performed a complete analysis of the C2HDM, using ML to explore the full parameter space and the observables that comply with current theoretical and experimental constraints. The ML method shown can be applied to any sampling in constrained scenarios, such as BSM models with a large number of parameters.

Part III.

Dark Matter Analysis in the NMSSM

As the SM leaves open questions like the nature of DM or why there is more matter than antimatter in the universe, we have to consider models beyond the SM. Among the many BSM theories, supersymmetry (SUSY) answers many of the open questions. Furthermore, it provides a relation between bosons and fermions through SUSY transformations. The scalar sector of the Minimal Supersymmetric extension of the SM (MSSM) contains two complex Higgs doublets, which are further extended in the NMSSM (c.f. Sec. 2.4) by a complex singlet superfield. This introduction solves the so-called μ -problem of the MSSM, but adds additional input parameters to the model. In SUSY, the tree-level mass of the lightest doublet-like CP-even Higgs boson has an upper limit, such that higher-order corrections are needed in order to comply with the measured Higgs boson mass of 125 GeV. Therefore, the mass of the Higgs boson is now a derived parameter. This, along with the large number of input parameters, makes parameter scans in the NMSSM difficult. Searching for benchmark scenarios that comply with all relevant theoretical and experimental constraints is particularly difficult due to the complexity of the parameter space.

To solve this problem, we developed **NMSSMScanner** [128], a framework that enables efficient scans of the NMSSM parameter space. To obtain valid parameter points, we include all relevant collider and low-energy constraints, as well as DM constraints. The framework is implemented using code that computes relevant NMSSM observables and compares them against theoretical and experimental constraints. One of these observables is the DM relic density and the direct-detection cross section of the potential DM candidate, here, the lightest neutralino $\tilde{\chi}_0$. To calculate these observables, we used the public code **Re1Ext** and, as part of this project, added the NMSSM as a new model to the toolchain.

In this chapter, we provide an overview of the formulas used to calculate the DM observables. This is followed in Ch. 10 by a brief description of the public code **Re1Ext** [129]. In Ch. 11, we will discuss the additional observables considered in **NMSSMScanner**. Afterwards, we will present our results in Ch. 12.

9.1. Dark Matter Relic Density in the NMSSM

The lightest neutralino $\tilde{\chi}_1^0$ is a promising DM candidate. In supersymmetric models, for many parameter configurations, it is the lightest stable supersymmetric particle (LSP). Note that, due to the imposed R -parity, it cannot decay further. The DM relic density for the MSSM has been calculated over the years [130–133]. In Ref. [133], it has been shown that the inclusion of co-annihilations between the lightest neutralino and other supersymmetric particles is necessary if they are close in mass. A full relic density calculation including all co-annihilation channels has been performed for the MSSM in Ref. [134]. The same procedure can be applied to the NMSSM. In Tab. 9.1, we list all processes involved in the calculation of the relic density in the NMSSM. In what follows, we show how to incorporate all channels into the Boltzmann equation. We will follow the description given in Ref. [134].

In Sec. 3.5, we derived the Boltzmann equation in order to calculate the relic density for a single DM candidate. Consider now N supersymmetric particles χ_i ($i \in [1, \dots, N]$) with masses m_i , where the masses are ordered as $m_1 \leq \dots \leq m_N$. The evolution of the number density n_i of the i -th particle is then described by

$$\begin{aligned} \frac{dn_i}{dt} = & -3Hn_i - \sum_{j=1}^N \langle \sigma_{ij} v_{ij} \rangle (n_i n_j - n_i^{\text{eq}} n_j^{\text{eq}}) \\ & - \sum_{j \neq i} [\langle \sigma_{Xij} v_{ij} \rangle (n_i n_X - n_i^{\text{eq}} n_X^{\text{eq}}) - \langle \sigma_{Xji} v_{ij} \rangle (n_j n_X - n_j^{\text{eq}} n_X^{\text{eq}})] \\ & - \sum_{j \neq i} [\Gamma_{ij} (n_i - n_i^{\text{eq}}) - \Gamma_{ji} (n_j - n_j^{\text{eq}})] , \end{aligned} \quad (9.1)$$

where v_{ij} is the relative velocity, which reads

$$v_{ij} = \frac{\sqrt{(p_i \cdot p_j)^2 - m_i^2 m_j^2}}{E_i E_j} \quad (9.2)$$

with p_i and E_i the four-momentum and energy of the particle χ_i , respectively. Furthermore, n_i^{eq} is the equilibrium number density of the particle χ_i , which is given by Eq. (3.41) upon inserting the equilibrium distribution function f_i^{eq} and the corresponding spin degrees of freedom g_i of the particle χ_i . The first term of Eq. (9.1) describes the expansion of the universe, where H is the Hubble parameter. The second term describes the annihilation of $\chi_i \chi_j$ into a final state f . Here, the total cross section is given by

$$\sigma_{ij} = \sum_f \sigma(\chi_i \chi_j \rightarrow f) . \quad (9.3)$$

The conversion process, which can occur by scattering off the cosmic background, of χ_i into χ_j , is described by the third term of Eq. (9.1). The cross section for these kinds of processes is given by

$$\sigma_{Xij} = \sum_Y \sigma(\chi_i X \rightarrow \chi_j Y) . \quad (9.4)$$

Here, X and Y denote standard model particles involved in the process. The last term of Eq. 9.1 describes the decay of the particle χ_i , where the decay rate is given by

$$\Gamma_{ij} = \sum_X \Gamma(\chi_i \rightarrow \chi_j X) . \quad (9.5)$$

The distribution functions in the Maxwell-Boltzmann approximation are given by

$$f_i = e^{-E_i/T} \quad (9.6)$$

Initial state	Final state
$\tilde{\chi}_i^0 \tilde{\chi}_j^0$	$h_k^0 h_l^0$ ($k, l \in [1, 2, 3]$), $A_i A_j$ ($i, j \in [1, 2]$), $H^\pm H^\mp$, $h_k^0 Z$, $H^\pm W^\mp$ ZZ , $W^+ W^-$, $\nu_a \bar{\nu}_a$, $\ell_a^+ \ell_a^-$, $u_a \bar{u}_a$, $d_a \bar{d}_a$ ($a \in [1, 2, 3]$)
$\tilde{\chi}_i^0 \tilde{\chi}_j^\pm$	$h_k^0 H^\pm$, $h_k^0 W^\pm$ ($k \in [1, 2, 3]$), $A_k H^\pm$, $A_k W^\pm$ ($k \in [1, 2]$), $H^\pm \gamma$, $H^\pm Z$, $\gamma W^\pm$, $Z W^\pm$, $\nu_a \ell_a^\pm$, $u_a d_a$ ($a \in [1, 2, 3]$)
$\tilde{\chi}_i^\pm \tilde{\chi}_j^\mp$	$h_k^0 h_l^0$ ($k, l \in [1, 2, 3]$), $A_i A_j$ ($i, j \in [1, 2]$), $H^\pm H^\mp$, $h_k^0 \gamma$, $h_k^0 Z$, $H^\pm W^\mp$ $\gamma \gamma$, γZ , ZZ , $W^+ W^-$ $\nu_a \bar{\nu}_a$, $\ell_a^+ \ell_a^-$, $u_a \bar{u}_a$, $d_a \bar{d}_a$ ($a \in [1, 2, 3]$)
$\tilde{\chi}_i^\pm \tilde{\chi}_j^\pm$	$H^\pm H^\pm$, $H^\pm W^\pm$, $W^\pm W^\pm$

Table 9.1.: Neutralino and chargino annihilation/co-annihilation channels.

and the thermally averaged cross section $\langle \sigma_{ij} v_{ij} \rangle$ reads

$$\langle \sigma_{ij} v_{ij} \rangle = \frac{\int d^3 p_i d^3 p_j f_i f_j \sigma_{ij} v_{ij}}{\int d^3 p_i d^3 p_j f_i f_j} . \quad (9.7)$$

All supersymmetric particles χ_i ($i \in [2, \dots, N]$) will eventually decay into the LSP χ_1 , which does not decay further due to R -parity conservation. Therefore, the number density of the lightest particle is simply given by the sum of the number densities of all supersymmetric particles

$$n_{\chi_1} \equiv n = \sum_{i=1}^N n_i . \quad (9.8)$$

Using this definition, the terms in the second and third line cancel in Eq. (9.1) such that the evolution of the number density n is given by

$$\frac{dn}{dt} = -3Hn - \sum_{i,j=1}^N \langle \sigma_{ij} v_{ij} \rangle (n_i n_j - n_i^{\text{eq}} n_j^{\text{eq}}) . \quad (9.9)$$

The scattering cross section σ_{Xij} in Eq. (9.4) and the annihilation cross section σ_{ij} given in Eq. (9.3) are of the same order, however, the scattering rate is much faster than the annihilation rate, as the background number density n_X is much larger than any of the supersymmetric number densities n_i . The reason is that the SM particles are relativistic, whereas the supersymmetric particles are non-relativistic and therefore Boltzmann-suppressed. Due

to the scattering processes, the SUSY particles stay in thermal equilibrium, which leads to the ratios being equal to their equilibrium values

$$\frac{n_i}{n} \simeq \frac{n_i^{\text{eq}}}{n^{\text{eq}}} . \quad (9.10)$$

Using this, we can rewrite Eq. (9.9) such that we get

$$\frac{dn}{dt} = -3Hn - \langle \sigma_{\text{eff}} v \rangle (n^2 - n_{\text{eq}}^2) , \quad (9.11)$$

where

$$\langle \sigma_{\text{eff}} v \rangle = \sum_{ij} \langle \sigma_{ij} v_{ij} \rangle \frac{n_i^{\text{eq}} n_j^{\text{eq}}}{n^{\text{eq}} n^{\text{eq}}} \equiv \langle \sigma v \rangle . \quad (9.12)$$

As described in Sec. (3.5), we can write the Boltzmann equation in terms of the yield $Y = \frac{n}{s}$, such that we obtain

$$\frac{dY}{dx} = -\sqrt{\frac{\pi}{45G}} \frac{g_*^{1/2} m_1}{x^2} \langle \sigma v \rangle (Y^2 - Y_{\text{eq}}^2) , \quad (9.13)$$

which can be solved for the yield Y_0 at the current temperature T_0 , so that we can use Eq. (3.69) to obtain the current relic density $\Omega_\chi h^2$.

9.1.1. Thermally Averaged Cross Section

Before we can actually solve Eq. (9.13), we first need to obtain an expression for the thermally averaged cross section $\langle \sigma v \rangle$. We first separate Eq. (9.12) into the numerator term A and the denominator n_{eq}^2 such that it reads

$$\langle \sigma v \rangle = \frac{\sum_{ij} \langle \sigma_{ij} v_{ij} \rangle n_i^{\text{eq}} n_j^{\text{eq}}}{n_{\text{eq}}^2} = \frac{A}{n_{\text{eq}}^2} . \quad (9.14)$$

The denominator is obtained by using the Boltzmann distribution function as

$$n_{\text{eq}}^2 = \left(\sum_i n_i^{\text{eq}} \right)^2 = \left(\sum_i \frac{g_i}{(2\pi)^3} \int d^3 p_i e^{-E_i/T} \right)^2 = \left(\frac{T}{2\pi^2} \sum_i g_i m_i^2 K_2 \left(\frac{m_i}{T} \right) \right)^2 . \quad (9.15)$$

Here, K_2 denotes the modified Bessel function of the second kind. The numerator A is given by

$$A = \sum_{ij} \langle \sigma_{ij} v_{ij} \rangle n_i^{\text{eq}} n_j^{\text{eq}} = \sum_{ij} \frac{g_i g_j}{(2\pi)^6} \int d^3 p_i d^3 p_j f_i f_j \sigma_{ij} v_{ij} , \quad (9.16)$$

which can be rewritten in a more convenient way as

$$A = \sum_{ij} \int W_{ij} \frac{g_i f_i d^3 p_i}{(2\pi)^3 2E_i} \frac{g_j f_j d^3 p_j}{(2\pi)^3 2E_j} , \quad (9.17)$$

where we introduced the quantity W_{ij} , which reads

$$W_{ij} = 4p_{ij} \sqrt{s} \sigma_{ij} = 4\sigma_{ij} \sqrt{(p_i \cdot p_j)^2 - m_i^2 m_j^2} = 4E_i E_j \sigma_{ij} v_{ij} . \quad (9.18)$$

Here, we defined the absolute value of the three-momentum of the particle χ_i in the center-of-mass (CM) frame of the pair $\chi_i \chi_j$ as $p_{ij} \equiv |\vec{p}_i| = |\vec{p}_j|$, which reads

$$p_{ij} = \frac{[s - (m_i + m_j)^2]^{1/2} [s - (m_i - m_j)^2]^{1/2}}{2\sqrt{s}} , \quad (9.19)$$

where s is the Mandelstam variable and is defined as

$$s = (p_i + p_j)^2 = (p_k + p_l)^2, \quad (9.20)$$

with the four-momenta of the initial state and final particles p_i, p_j and p_k, p_l , respectively. The energy of the particle χ_i is denoted by E_i . For an n -body final state, we can write the contribution of W_{ij} , after averaging over initial states and summing over all final states f , as

$$W_{ij}^{\text{n-body}} = \frac{1}{g_i g_j S_f} \sum_{\text{internal d.o.f}} \int |\mathcal{M}|^2 (2\pi)^4 \delta^4(p_i + p_j - \sum_f p_f) \prod_f \frac{d^3 p_f}{(2\pi)^3 2E_f}. \quad (9.21)$$

Here S_f denotes the symmetry factor accounting for identical particles, and g_i are the spin degrees of freedom of the particle χ_i , and $\mathcal{M}$ denotes the scattering amplitude. In the case of the $2 \rightarrow 2$ processes in the form of $ij \rightarrow kl$ this simplifies to

$$W_{ij \rightarrow kl} = \frac{p_{kl}}{16\pi^2 g_i g_j S_{kl} \sqrt{s}} \sum_{\text{internal d.o.f}} \int |\mathcal{M}(ij \rightarrow kl)| d\Omega. \quad (9.22)$$

In Eq. (9.22), p_{kl} denotes the absolute value of the CM three-momentum of the final states, S_{kl} equals 2 for identical final state particles or 1 otherwise. Furthermore, we are integrating over the solid angle between the final-state particles. Next, we will reduce the six-dimensional integral of Eq. (9.17) to a one-dimensional integral. First, we specify for the distribution functions the Boltzmann distribution such that Eq. (9.17) becomes

$$A = \sum_{ij} \int g_i g_j W_{ij} e^{-E_i/T} e^{-E_j/T} \frac{d^3 p_i}{(2\pi)^3 2E_i} \frac{d^3 p_j}{(2\pi)^3 2E_j}, \quad (9.23)$$

where T is the temperature. The phase-space integration measure $\frac{d^3 p_i}{(2\pi)^3 2E_i} \equiv d\Pi_i$ can be rewritten in terms of the angle γ between the initial state momenta p_i and p_j and their energies E_i and E_j such that it reads

$$d\Pi_i d\Pi_j = \frac{1}{2(2\pi)^4} |\vec{p}_i| |\vec{p}_j| dE_i dE_j d\cos\gamma. \quad (9.24)$$

Following the derivation given in Ref. [134], we can perform a variable transformation that reads

$$\begin{cases} E_+ = E_i + E_j \\ E_- = E_i - E_j \\ s = m_i^2 + m_j^2 + 2E_i E_j - 2|\vec{p}_i| |\vec{p}_j| \cos\gamma, \end{cases} \quad (9.25)$$

such that the integration measure in Eq. (9.24) becomes

$$d\Pi_i d\Pi_j = \frac{1}{(2\pi)^4} \frac{dE_+ dE_- ds}{8}. \quad (9.26)$$

The integration regions are then given by

$$s \geq (m_i + m_j)^2 \quad (9.27a)$$

$$E_+ \geq \sqrt{s} \quad (9.27b)$$

$$\left| E_- - E_+ \frac{m_j^2 - m_i^2}{s} \right| \leq 2p_{ij} \sqrt{\frac{E_+^2 - s}{s}}. \quad (9.27c)$$

As Eq. (9.23) does not depend on E_- , the integration can be trivially performed, for which then the integration measure is given by

$$d\Pi_i d\Pi_j = \frac{p_{ij}}{2(2\pi)^4} \sqrt{\frac{E_+^2 - s}{s}} dE_+ ds. \quad (9.28)$$

Inserting Eq. (9.28) in Eq. (9.23) and integrating over E_+ , we then obtain

$$A = \frac{T}{32\pi^2} \sum_{ij} \int_{(m_i+m_j)^2}^{\infty} p_{ij} W_{ij} K_1 \left(\frac{\sqrt{s}}{T} \right) ds. \quad (9.29)$$

Finally, after inserting Eqs. (9.29) and (9.15) in Eq. (9.14), we obtain the following expression for the thermally averaged cross section

$$\langle \sigma v \rangle = \frac{\sum_{i,j} \int_{(m_i+m_j)^2}^{\infty} p_{ij} W_{ij} K_1 \left(\frac{\sqrt{s}}{m_{\chi_1}} x \right) ds}{8T \left(\sum_i g_i m_i^2 K_2 \left(\frac{m_i}{m_{\chi_1}} x \right) \right)^2}, \quad (9.30)$$

where we substituted the temperature in the Bessel functions with $T = \frac{x}{m_{\chi_1}}$.

9.2. Direct Detection in the NMSSM

After reviewing the calculation of the DM relic density in the NMSSM in the last section, we now turn our attention to the calculation of the direct-detection cross section. In the following, we will follow the description given in Ref. [135]. The formulas presented here have been used to calculate the direct-detection cross section in this work.

In order to obtain the direct-detection cross section in the NMSSM, we first give the most general supersymmetric effective four-fermion Lagrangian, which reads

$$\begin{aligned} \mathcal{L}_{\text{eff}} = & \bar{\chi}_1^0 \gamma^\mu \gamma_5 \tilde{\chi}_1^0 \bar{q}_i \gamma_\mu (\alpha_{1i} + \alpha_{2i} \gamma_5) q_i + \alpha_{3i} \bar{\chi}_1^0 \tilde{\chi}_1^0 \bar{q}_i q_i \\ & + \alpha_{4i} \bar{\chi}_1^0 \gamma_5 \tilde{\chi}_1^0 \bar{q}_i \gamma_5 q_i + \alpha_{5i} \bar{\chi}_1^0 \tilde{\chi}_1^0 \bar{q}_i \gamma_5 q_i + \alpha_{6i} \bar{\chi}_1^0 \gamma_5 \tilde{\chi}_1^0 \bar{q}_i q_i. \end{aligned} \quad (9.31)$$

Here, the index i ($i \in [1, 2]$) distinguishes between up- and down-type quarks, and the summation over the three quark generations is assumed implicitly. The couplings α_{1i} , α_{4i} , α_{5i} , and α_{6i} are velocity-suppressed and can therefore be neglected in the scope of this work. Furthermore, the α_{2i} term contributes to the spin-dependent case, while the α_{3i} term contributes to the spin-independent case. As we are interested in the spin-independent cross section, we will focus on the α_3 term in the following. In Fig.9.1, we show the generic diagrams which contribute to the α_{3i} term. The left diagram depicts the s -channel exchange with a squark mediator, and the right diagram depicts the t -channel exchange with a neutral Higgs propagator. Accordingly, we can write α_{3i} as a sum of both contributions

$$\alpha_{3i} = \alpha_{3i}^{\tilde{q}} + \alpha_{3i}^h. \quad (9.32)$$

Here the $\alpha_{3i}^{\tilde{q}}$ denotes the squark contributions and α_{3i}^h denotes the Higgs contributions. The terms read as

$$\alpha_{3i}^{\tilde{q}} = - \sum_{X=1}^2 \frac{1}{4(m_{X_i}^2 - m_{\tilde{\chi}_1^0}^2)} \text{Re} \left[(C_R^{X_i})(C_L^{X_i}) \right], \quad (9.33)$$

$$\alpha_{3i}^h = \sum_{a=1}^3 \frac{1}{m_{h_a^0}^2} (C_Y^i) \text{Re} [(C_{HL}^a)] . \quad (9.34)$$

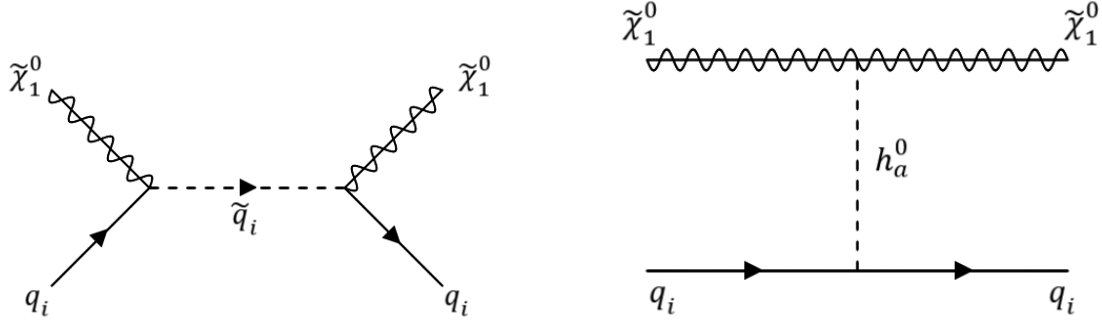


Figure 9.1.: Generic diagrams contributing to the direct-detection cross section in the NMSSM. Left: s -channel exchange with a squark $\tilde{q}_i$ ($i \in [1, 2]$) mediator. Right: t -channel exchange with a neutral scalar h_a^0 ($a \in [1, 2, 3]$) mediator.

Here X ($X \in [1, 2]$) denote the squark mass eigenstates and h_a^0 ($a \in [1, 2, 3]$) denote the neutral scalar mass eigenstates. We provide the couplings for the squark-quark-neutralino ($C_{R,L}^{X_i}$), neutralino-neutralino-Higgs (C_{HL}^a) and the Higgs-quark-quark interaction C_Y^i in Appendix A. Recalling Eq. (3.85) and assuming a neutralino-proton interaction, the cross section is given by¹²

$$\sigma_{\text{SI}}^p = \frac{4m_\chi}{\pi} c_{s,p}^2. \quad (9.35)$$

The scalar Wilson coefficient for the DM-proton interaction in the NMSSM is then given by Eq. (3.79) by setting $c_{s,q} = \alpha_{3q}$. To compare with the experimental exclusion bounds of the LUX-Zeplin experiment, we calculate the normalized spin-independent direct-detection cross section (SI-DD) $\sigma_{\text{SI-DD}}$ as follows

$$\sigma_{\text{SI-DD}} = \frac{Z_{\text{Xe}} \sigma_{\text{SI}}^p + (A_{\text{Xe}} - Z_{\text{Xe}}) \sigma_{\text{SI}}^n}{A_{\text{Xe}}}, \quad (9.36)$$

where Z_{Xe} and A_{Xe} are the proton and atomic number of Xenon. However, the exclusion line assumes the relic density given in Eq. (3.22). We allow points with relic abundances lower than the measured value. Therefore, to compare our results with the DD limits from experimental measurement, we normalize the SI-DD cross section such that it reads

$$\sigma_{\text{SI-DD-N}} \equiv \sigma_{\text{SI-DD}} \frac{\Omega_c h^2}{\Omega_{\text{exp}} h^2}. \quad (9.37)$$

Here, $\Omega_{\text{exp}} h^2$ is given in Eq. (3.22) and $\Omega_c h^2$ denotes the calculated relic density for the model and parameter point. To calculate both the relic density and the direct-detection cross section, we implemented the NMSSM in our public code `RelExt`. In the next chapter, we will provide an overview of the code.

¹²The cross section for DM-neutron scattering is obtained analogously, replacing $p \rightarrow n$.

RelExt - A Dark Matter Tool for Efficient Scans

Calculating DM observables such as the relic density and the direct-detection cross section can be tedious in a BSM model like the NMSSM. Over the years, many codes like **MadDM** [136–138], **DarkSUSY** [139], **SuperISO** [140] and **MicrOMEGAs** [66, 141–145] have been developed to calculate DM observables. However, finding the appropriate input parameter configuration to achieve the relic abundance given in Eq. (3.22) for an arbitrary model becomes harder as the model grows more complex. To overcome this problem, we developed the public code **RelExt**, which calculates the relic density and includes a scanning tool that efficiently searches for parameter values that yield the correct relic density. Furthermore, we have extended the code to implement direct-detection in the NMSSM. Also, it is possible to evaluate the relic density calculation not only at tree level but also at next-to-leading order (NLO), which we will showcase in Part IV for the CxSM. The code can be downloaded at

<https://github.com/jplotnikov99/RelExt>.

RelExt is a C++ code, which calculates the relic density for DM particles that undergo the freeze-out mechanism described in Sec. 3.5 for any model with a $\mathbb{Z}_2$ symmetry, which stabilizes the DM particle. In order to run the code, the user only needs to provide a **FeynRules** [146] model file. **RelExt** then calculates all (co-)annihilation amplitudes of the DM candidate of the given model, generates the corresponding cross sections, and calculates with that the thermally averaged cross section given in Eq. (9.30). The relic density is then obtained by solving the Boltzmann equation given in Eq. (3.66). For a more detailed description of the implementation of the C++ code, we refer to Ref. [129]. Note that in the current version of **RelExt**, it is only possible to work with models that have one DM candidate. Furthermore, BSM theories with DM annihilation processes that are CP-violating and enter the relic density calculation, cannot be described by the derivation given in Sec. 3.5, and hence, cannot be treated in **RelExt**. In this work, we provide a brief overview of the structure of the code. Afterwards, we show how we implement the calculation of the direct-detection cross section in **RelExt**.

In Figure 10.1, we show the flowchart of the code. **RelExt** can be divided into two parts. We denote the first part as **New Model Implementation** and the second part as **DM Observables and Parameter Search**. We will start our description with the former.

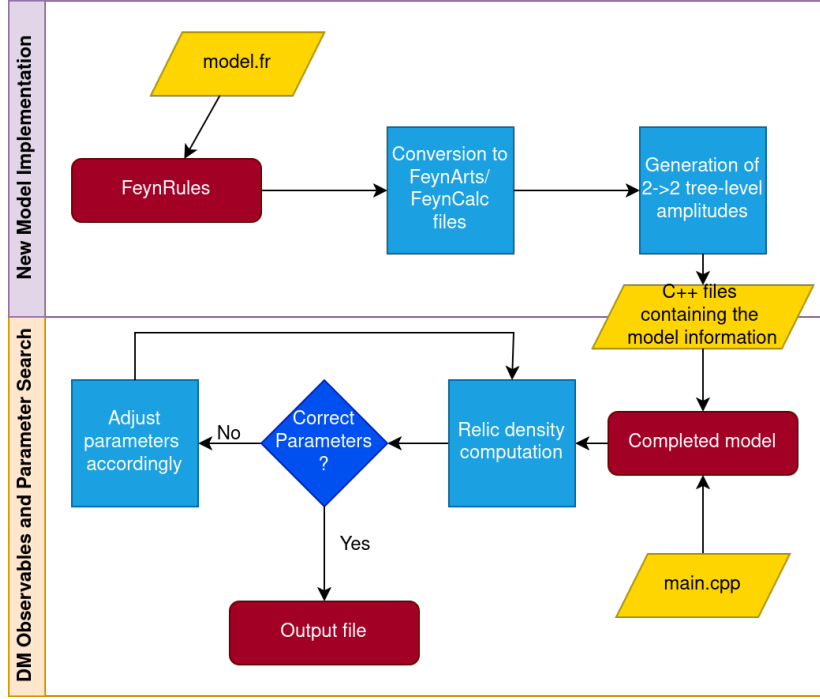


Figure 10.1.: Flowchart of the code RelExt. Taken from Ref. [129].

10.1. New Model Implementation

If the user wants to implement a new model in RelExt, they have to provide a FeynRules model file. RelExt is then able to generate automatically the FeynArts [147,148] and FeynCalc [149,150] model files. Implemented in RelExt is also a Mathematica code, which uses the generated FeynArts and FeynCalc files to generate all relevant $2 \rightarrow 2$ (co-)annihilation amplitudes. Furthermore, it generates all relevant information for the model, such as decay channels and resonances, that appear in s -channel diagrams. Afterwards, the generated squared amplitudes of the Mathematica code are converted into C++ files, which are then used in the second part of the code. A detailed overview of the important functions of the Mathematica code is given in App. B.1.

Generation of the Annihilation Amplitudes

In order to calculate the DM relic abundance, we first generate all $2 \rightarrow 2$ (co-)annihilation amplitudes. The code automatically identifies all dark sector particles in the model and then generates all possible amplitudes with any combination of two dark sector particles in the initial state and two visible particles in the final state. These are generated by FeynCalc. As we integrate over the thermally averaged cross section in terms of the Mandelstam variable s , we may encounter divergences arising from s -channel propagators. These divergences are cured by introducing an imaginary part in terms of the decay width of the intermediate particle in the propagator, such that it reads

$$\frac{1}{s - m_{\text{med}}^2} \rightarrow \frac{1}{s - m_{\text{med}}^2 + i\Gamma_{\text{med}}m_{\text{med}}} , \quad (10.1)$$

where m_{med} and Γ_{med} denote the mass and the decay width of the mediator particle, respectively. Here, the code automatically identifies all possible s -channel mediators and Afterwards calculates their decay widths. Note that it is also possible to encounter t - and u -channel divergences. Here, we use a similar approach as in MicrOMEGAs and introduce a regulator width Γ_i which is given by

$$\Gamma_i = \frac{m_i}{1000} , \quad (10.2)$$

$\overline{m}_b(\overline{m}_b)$	$\overline{m}_c(3 \text{ GeV})$	$\overline{m}_s(2 \text{ GeV})$
4.18 GeV	0.986 GeV	0.095 GeV

Table 10.1.: Input values of the $\overline{\text{MS}}$ quark masses $\overline{m}_i(Q)$ at the scale Q . The values are taken from Ref. [152].

where the subscript denotes the mediator particle i . Using this width, we obtain up to 1% deviation from the result with zero width outside the divergent region. In the case of DM annihilation into quarks, we use running quark masses in the final states, except for the top quark, where we use the pole mass value. This value is given by the user. The running masses are computed at next-to-next-to-next-to leading log accuracy (N³LL) [151]. The mass values are evolved from the input scale to the characteristic scale of the DM annihilation process, which we set to twice the DM mass. The $\overline{\text{MS}}$ mass values $\overline{m}_i(Q)$ ($i \in [s, c, b]$) at the scale Q are provided in Tab. 10.1. The masses of the first-generation quarks and the leptons must be provided by the user. In DM (co-)annihilation processes, we use the strong coupling constant α_s at the scale given by twice the DM masses. In the computation of the decay widths, we compute the strong coupling constant at the scale given by the mass of the decaying particle. The evaluation of the strong coupling is done at next-to-next-to-next-to leading order (N³LO) [151].

The expressions for the squared amplitudes obtained from the `Mathematica` code are automatically converted into `C++` code. Note that at this stage, no spin or color average factors are included in these squared amplitudes. They are included at a later stage in the cross section calculations.

Computation of the Total Decay Widths

In this section, we briefly describe how we compute the total decay widths introduced in Eq. (10.1). The code automatically calculates the total decay width as the sum of all partial decay widths of the mediator particle. All decay widths are calculated for $1 \rightarrow 2$ decays and at leading order, apart from scalar and pseudoscalar particles.

As the decay widths of the SM gauge bosons $V = W^\pm, Z$ are measured with very high precision experimentally, we take their decay widths from the input model files, if they act as mediator particles. In case of the top quark, `ReLExT` calculates the decay width automatically.¹³ The total decay widths of all other mediator particles are obtained by calculating and summing all tree-level partial decay widths.

For scalar and pseudoscalar mediators, we include the dominant available higher-order corrections. Here, we follow the implementation of `HDECAY` [153, 154], a code that calculates the decay widths of Higgs bosons for the SM and the MSSM, and where state-of-the-art higher-order corrections are included. We follow the description given in Ref. [151], unless stated otherwise. In our computation, we include the coupling modifiers of the scalar or pseudoscalar mediator to SM particles, as specified by the given model. In the case of leptonic decays, we take the tree-level formula, which reads

$$\Gamma(\Phi \rightarrow l\bar{l}) = \frac{G_F m_\Phi}{4\sqrt{2}\pi} (c_l^\Phi)^2 m_l^2 \left(1 - \frac{4m_l^2}{m_\Phi^2}\right)^{p/2}, \quad (10.3)$$

¹³We emphasize that this could lead to a total top decay width, which does not comply with the experimental measurement. The user must ensure that the chosen parameter configuration for the model does not violate the experimental constraints.

where G_F denotes the Fermi constant, m_Φ and m_l are the masses of the mediator particle Φ and the lepton l , respectively. In Eq. (10.3), c_l^Φ denotes the model-specific coupling modifier of the decaying particle to leptons and $p = 3(1)$ for scalar (pseudoscalar) Higgs bosons. For quark decays, we include higher-order QCD corrections. Here, we use the interpolation between the large Higgs-mass region and the threshold region, i.e., $m_\Phi \approx 2m_Q$. The decay width into quarks Q is then, for the large Higgs-mass case, given by

$$\Gamma(\Phi \rightarrow Q\bar{Q}) = \frac{3G_F m_\Phi}{4\sqrt{2}\pi} \bar{m}_Q^2(m_\Phi) (c_Q^\Phi)^2 (1 + \delta_{\text{QCD}} + \delta_t^\Phi). \quad (10.4)$$

Here, $\bar{m}_Q(m_\Phi)$ is the $\overline{\text{MS}}$ quark mass at the scale given at m_Φ , c_Q^Φ denotes the coupling modifier of the decaying particle to quarks. The QCD corrections δ_{QCD} reads

$$\begin{aligned} \delta_{\text{QCD}} = & 5.67 \frac{\alpha_s(m_\Phi)}{\pi} + (35.94 - 1.36N_F) \left(\frac{\alpha_s(m_\Phi)}{\pi} \right)^2 \\ & + (164.14 - 25.77N_F + 0.259N_F^2) \left(\frac{\alpha_s(m_\Phi)}{\pi} \right)^3, \end{aligned} \quad (10.5)$$

where $N_F = 5$ denotes the number of contributing quark flavors and the running strong coupling $\alpha_s(Q)$ is taken at the scale of the decaying particles, i.e. $Q = m_\Phi$, which absorbs large logarithms. The relative top-quark induced corrections δ_t^Φ for a scalar particle h are given by

$$\delta_t^h = \frac{c_t^h}{c_Q^h} \left(\frac{\alpha_s(m_h)}{\pi} \right)^2 \left[1.57 - \frac{2}{3} \log \frac{m_h^2}{m_t^2} + \frac{1}{9} \log^2 \frac{\bar{m}_Q^2(m_h)}{m_h^2} \right], \quad (10.6)$$

and for a pseudoscalar particle A , it reads

$$\delta_t^A = \frac{c_t^A}{c_Q^A} \left(\frac{\alpha_s(m_A)}{\pi} \right)^2 \left[3.83 - \log \frac{m_A^2}{m_t^2} + \frac{1}{6} \log^2 \frac{\bar{m}_Q^2(m_A)}{m_A^2} \right]. \quad (10.7)$$

Finite quark masses become relevant in the threshold region. In this case, we use the following relation for the decay

$$\Gamma(\Phi \rightarrow Q\bar{Q}) = \frac{3G_F m_\Phi}{4\sqrt{2}\pi} (c_Q^\Phi)^2 m_Q^2 \left(1 - \frac{4m_Q^2}{m_\Phi^2} \right)^{p/2} \left(1 + \frac{4\alpha_s(m_\Phi)}{3\pi} \delta^\Phi \right). \quad (10.8)$$

Here, the QCD corrections δ^Φ for the scalar case is given by

$$\delta^h = \frac{1}{\beta} A(\beta) + \frac{1}{16\beta^3} (3 + 34\beta^2 - 13\beta^4) \log \left(\frac{1+\beta}{1-\beta} \right) + \frac{3}{8\beta^2} (7\beta^2 - 1), \quad (10.9)$$

where $\beta = (1 - 4m_q^2/m_h^2)^{1/2}$. The QCD corrections for the pseudoscalar case read

$$\delta^A = \frac{1}{\beta} A(\beta) + \frac{1}{16\beta} (19 + 2\beta^2 + 3\beta^4) \log \left(\frac{1+\beta}{1-\beta} \right) + \frac{3}{8} (7 - \beta^2), \quad (10.10)$$

with $\beta = (1 - 4m_q^2/m_A^2)^{1/2}$. In Eqs. (10.9) and (10.10), we introduced the function $A(\beta)$, which reads

$$\begin{aligned} A(\beta) = & (1 + \beta^2) \left[4\text{Li}_2 \left(\frac{1-\beta}{1+\beta} \right) + 2\text{Li}_2 \left(-\frac{1-\beta}{1+\beta} \right) - 3 \log \left(\frac{1+\beta}{1-\beta} \right) \log \left(\frac{2}{1+\beta} \right) \right. \\ & \left. - 2 \log \left(\frac{1+\beta}{1-\beta} \right) \log(\beta) \right] - 3\beta \log \left(\frac{4}{1-\beta^2} \right) - 4\beta \log(\beta). \end{aligned} \quad (10.11)$$

In the threshold region, we always use pole quark masses, and thus do not perform a running of the masses, for all quark flavors. For the partial decay widths into gluons at leading order, we use the following equation for the scalar case

$$\Gamma_{\text{LO}}(h \rightarrow gg) = \frac{G_F \alpha_s^2 m_h^3}{36\sqrt{2}\pi^3} \left| \sum_Q c_Q^h A_Q^h(\tau_Q) \right|^2, \quad (10.12)$$

where $\tau_Q = 4m_Q^2/m_h^2$ and $A^h(\tau)$ is given by

$$A_Q^h(\tau) = \frac{3\tau}{2} (1 + (1 - \tau)f(\tau)). \quad (10.13)$$

The function $f(\tau)$ reads

$$f(\tau) = \begin{cases} \arcsin^2\left(\frac{1}{\sqrt{\tau}}\right) \\ -\frac{1}{4} \left[\log\left(\frac{1 + \sqrt{1 - \tau}}{1 - \sqrt{1 - \tau}}\right) - i\pi \right]^2 \end{cases}. \quad (10.14)$$

The pseudoscalar leading-order decay width into gluons is given by

$$\Gamma_{\text{LO}}(A \rightarrow gg) = \frac{G_F \alpha_s^2 m_A^3}{16\sqrt{2}\pi^3} \left| \sum_Q c_Q^A A_Q^A(\tau_Q) \right|^2, \quad (10.15)$$

with

$$A_Q^A(\tau) = \tau f(\tau). \quad (10.16)$$

The higher-order QCD corrections up to N³LO for the scalar case and five quark flavours N_F are given by

$$\begin{aligned} \Gamma(h \rightarrow gg) = & \Gamma_{\text{LO}}(h \rightarrow gg) \left[1 + (23.75 - 1.167N_F + \Delta_m) \frac{\alpha_s(m_h)}{\pi} \right. \\ & + \left(370.20 - 47.19N_F + 0.902N_F^2 + (2.375 + 0.667N_F) \log\left(\frac{m_h^2}{m_t^2}\right) \right) \\ & \times \left(\frac{\alpha_s(m_h)}{\pi} \right)^2 + \left(4533.46 - 1062.82N_F + 52.62N_F^2 - 0.5378N_F^3 + \right. \\ & \left. (66.66 + 14.6N_F - 0.6887N_F^2) \log\left(\frac{m_h^2}{m_t^2}\right) + (6.53 + 1.44N_F - 0.111N_F^2) \right. \\ & \left. \times \log^2\left(\frac{m_h^2}{m_t^2}\right) \right) \left(\frac{\alpha_s(m_h)}{\pi} \right)^3 \left. \right], \end{aligned} \quad (10.17)$$

where Δ_m denotes the next-to-leading-order quark mass effects from the top, bottom and charm quarks [155]. In the pseudoscalar scenario, the QCD higher-order corrections have been calculated up to next-to-next-to-leading order and take the form

$$\begin{aligned} \Gamma(A \rightarrow gg) = & \Gamma_{\text{LO}}(A \rightarrow gg) \left\{ 1 + (24.25 - 1.167N_F + \Delta_m) \frac{\alpha_s(m_A)}{\pi} \right. \\ & + \left(392.22 - 48.58N_F + 0.888N_F^2 + N_F \log\frac{m_A^2}{m_t^2} \right) \left(\frac{\alpha_s(m_A)}{\pi} \right)^2 \left. \right\}. \end{aligned} \quad (10.18)$$

Off-shell decays into massive gauge bosons $V = W^\pm, Z$ are included in the computation of the total width. These are allowed only in a CP-conserving theory with scalar mediators.

We consider two cases, where the center-of-mass energy is larger than twice the gauge boson mass, $m_h \geq 2m_V$, and where the energy is smaller than m_V , i.e., $m_h \leq m_V$. In the case of the former, we use the following relations for the on-shell decay into gauge bosons

$$\Gamma(h \rightarrow ZZ) = \frac{G_F m_h^3}{16\sqrt{2}\pi} \left(1 - 4\frac{m_Z^2}{m_h^2}\right)^{1/2} \left(1 - 4\frac{m_Z^2}{m_h^2} + 12\left(\frac{m_Z^2}{m_h^2}\right)^2\right), \quad (10.19)$$

and

$$\Gamma(h \rightarrow WW) = \frac{2G_F m_h^3}{16\sqrt{2}\pi} \left(1 - 4\frac{m_W^2}{m_h^2}\right)^{1/2} \left(1 - 4\frac{m_W^2}{m_h^2} + 12\left(\frac{m_W^2}{m_h^2}\right)^2\right). \quad (10.20)$$

Here, we do not include QCD corrections, as they are negligible, and also it ensures a smooth transition to the off-shell decays, where the QCD corrections are not available in a compact form. In the energy range of $m_h \leq m_V$, we use the following relation

$$\Gamma(h \rightarrow V^*V^*) = \frac{1}{\pi^2} \int_0^{m_h^2} \frac{dQ_1^2 m_V \Gamma_V}{(Q_1^2 - m_V^2)^2 + m_V^2 \Gamma_V} \int_0^{(m_h - Q_1)^2} \frac{dQ_2^2 m_V \Gamma_V}{(Q_2^2 - m_V^2)^2 + m_V^2 \Gamma_V} \Gamma_0, \quad (10.21)$$

where m_V and Γ_V denote the mass and the total decay width of the massive gauge boson $V = W^\pm, Z$, and $Q_i^2 (i \in [1, 2])$ are the squared invariant masses of the virtual gauge bosons. Further, Γ_0 reads

$$\Gamma_0 = \delta_V \frac{G_F m_h^3}{16\sqrt{2}\pi} \sqrt{\lambda(Q_1^2, Q_2^2, m_h^2)} \left[\lambda(Q_1^2, Q_2^2, m_h^2) + 12 \frac{Q_1^2 Q_2^2}{m_h^4} \right], \quad (10.22)$$

where $\delta_V = 2(1)$ for $V = W(Z)$ and $\lambda(x, y, z)$ denotes the Källén function, which is given by

$$\lambda(x, y, z) = \left(1 - \frac{x}{z} - \frac{y}{z}\right)^2 - \frac{4xy}{z^2}. \quad (10.23)$$

In the mass range $m_V \leq m_h \leq 2m_V$, we compute the decay where one gauge boson is on-shell and the other is off-shell. The relation used here is given by [156]

$$\Gamma(h \rightarrow VV^*) = \delta'_V \frac{3G_F^2 m_V^4 m_h}{16\pi^3} R\left(\frac{m_V^2}{m_h^2}\right). \quad (10.24)$$

Here, $\delta'_W = 1$ and $\delta'_Z = 7/12 - 10\sin^2(\theta_W)/9 + 40\sin^4(\theta_W)/27$ and the function $R(x)$ is given by

$$R(x) = \frac{3(1 - 8x + 20x^2)}{\sqrt{4x - 1}} \arccos\left(\frac{3x - 1}{2x^{3/2}}\right) - \frac{1 - x}{2x} (2 - 13x + 47x^2) - \frac{3}{2} (1 - 6x + 4x^2) \log(x). \quad (10.25)$$

Currently, we do not include the decays of a Z boson and photon or into a photon pair in our calculation. This is motivated by the fact that the partial decay widths are small and do not significantly alter the total width. Additionally, we also consider Higgs decays into new BSM particles. These can be, for example, decays into one lighter Higgs bosons plus a gauge boson, lighter Higgs boson pairs, or new heavy fermion or heavy gauge boson pairs. RelExt calculates all possible $1 \rightarrow 2$ non-SM-like decays and adds them to the total decay width of the mediating particle.

This concludes the description of the first part **New Model Implementation** of the code. Next, we will briefly describe the second part **DM Observables and Parameter Search**.¹⁴

¹⁴Note that we will not discuss the Parameter Search algorithms in this thesis. We refer for a more detailed overview on these to Ref. [129, 157].

10.2. DM Observables

With the previously generated C++ code for the squared amplitudes and decay widths, the DM observables, such as the thermally averaged cross section, the relic density, and the direct-detection cross section, are calculated. We start our description with the thermally averaged cross section.

Calculation of the Thermally Averaged Cross Section

In order to calculate the thermally averaged cross section given in Eq. (9.30), we first need to compute the cross section for a process of two dark sector particles i, j into a two-body final state k, l , which reads

$$\sigma_{ij} = \frac{1}{32\pi s g_i g_j} \sum_{k,l} \frac{\lambda^{1/2}(s, m_k^2, m_l^2)}{\lambda^{1/2}(s, m_i^2, m_j^2)} \int |\mathcal{M}_{ij \rightarrow kl}|^2 d\cos\theta. \quad (10.26)$$

Here, θ denotes the azimuthal scattering angle in the CM frame with respect to the axis of the incoming particles and $\mathcal{M}_{ij \rightarrow kl}$ is the (co-)annihilation matrix element. In the C++ code, we use a composite Simpson's 3/8 rule to obtain a rough estimate of the value. This estimate is used as a termination criterion of the adaptive Simpson's 3/8 method [158], which we use to calculate the cross section. This criterion is necessary to ensure rapid convergence, even in regions where the integrand is numerically small. After obtaining the cross section, we can now calculate the integral in Eq. (9.30). As in the calculation for the cross section, we first compute an estimate using the Kronrod 61-point method [158] for regions outside s -channel resonances. Again, this estimate is used as a termination criterion for the actual integration, which is performed using an adaptive Gauss-Kronrod 15-point method [158]. To cover the case when the sum of the final-state masses $m_k + m_l$ is larger than the sum of initial-state masses $m_i + m_j$, we adjust the lower integration boundary of Eq. (9.30) to $\max(m_i + m_j, m_k + m_l)$ to ensure that the integration is performed correctly over the available phase space. We do not consider channels that are Boltzmann suppressed, i.e., that do not fulfill the following condition

$$B = e^{-x \frac{m_{i(k)} + m_{i(l)} - 2m_\chi}{m_\chi}} > B_\epsilon. \quad (10.27)$$

Here, m_χ denotes the mass of the DM candidate, $x = \frac{m_\chi}{T}$ and B_ϵ is a numerical lower bound, which we set to $B_\epsilon = 10^{-6}$. As integrating over resonance peaks is numerically challenging, we integrate these regions separately if the following condition is fulfilled

$$e^{-x \frac{m_{\text{med}} - m_{i(k)} + m_{j(l)}}{m_\chi}} > B_\epsilon. \quad (10.28)$$

In this case, the peaks are determined by integrating this region with high precision using an adaptive Simpson's 3/8 method.

Computation of the Boltzmann Equation

After obtaining the thermally averaged cross section, we can finally compute the solution of Eq. (9.13). For this calculation, we use the interpolated values for the effective degrees of freedom g_{eff} , h_{eff} , and $g_*^{1/2}$ from Ref. [159]. Further, we compute the freeze-out point $x = x_f$ with the following condition [159]

$$\sqrt{\frac{\pi}{45G}} \frac{g_*^{1/2} m_\chi}{x^2} \langle \sigma v \rangle Y_{\text{eq}} \delta(\delta + 2) + \frac{d \ln(Y_{\text{eq}})}{dx} = 0. \quad (10.29)$$

Here, δ is a free parameter, that can be chosen arbitrarily. In order to find the freeze-out point x_f , we use a bisection method to find the root of the equation. In our code, we have implemented an option called **Fast**, which, when set to true, sets the parameter $\delta = 1.5$ [159]. The yield is then obtained by the freeze-out approximation, which reads

$$\frac{1}{Y_0} = \frac{1}{2.5Y_{\text{eq}}(x_f)} + \sqrt{\frac{\pi}{45G}} \int_{x_f}^{x_0} dx \frac{g_*^{1/2} m}{x^2} \langle \sigma v \rangle_{\text{eff}}, \quad (10.30)$$

where $x_0 = m_\chi/T_0$ and T_0 is the temperature of the universe today. In the approximation given in Eq. (10.30), the Y_{eq}^2 term is neglected.¹⁵ When the option **Fast** is set to false, we use $\delta = 0.1$. In this case, we solve Eq. (9.13) numerically, with a Dormand-Prince 853 method as described in Ref. [158]. Here, we set the initial condition $Y_f = 1.1Y_{\text{eq}}(x_f)$ at the freeze-out point.

Computation of the Direct-Detection Cross section

RelExt has been extended to compute spin-independent direct-detection cross sections. A new function `CalcDDT(slhFilePath, relic)` is added to the code, which computes the SI DM-Xenon scattering cross section in units of pb. In addition, the SI cross sections for DM-proton, DM-neutron, and DM-Xenon scattering, together with the corresponding exclusion limit obtained from the LUX-Zeplin Collaboration evaluated at the neutralino mass $m_{\tilde{\chi}_0}$, are written to the user-provided SLHA file. A detailed description of the implemented `DDetection` class is provided in Appendix B.2. A typical `main` routine of RelExt to compute both the relic density and the DD cross section will then look like the following:

```

1 int main(int argc, char **argv) {
2     Main M(argv, MODE, BEPS, XTODAY, FAST, CALCWIDTHS, SAVECONTRIBS);
3     M.set_channels(CONSIDERCHANNELS, NEGLECTCHANNELS, NEGLECTPARTICLES);
4
5     clock_t begin_time = clock();
6
7     M.LoadParameters(std::string(argv[1]));
8     double omega = M.CalcRelic();
9
10    M.LoadParameters(std::string(argv[2]));
11    M.CalcDDT(std::string(argv[2]), omega);
12
13    // M.SaveData(SAVEPARS);
14
15    std::cout << "Computation time:\n"
16              << float(clock() - begin_time) / CLOCKS_PER_SEC << std::endl;
17 }
```

After compiling the code, the command line to execute the program is

```
./NMSSM path/to/slh_CNMSM path/to/slh_NMSSM
```

Here, the user has to provide two SLHA input files: one in the format of the CP-violating NMSSM (`slha_CNMSM`) and one in the format of the CP-Conserving NMSSM (`slha_NMSSM`). While the two contain the numerical values specifying the same parameter point, the relic density can only be calculated with an SLHA file in the format of the CP-violating NMSSM, while the direct-detection cross section can only be calculated with an SLHA input in the

¹⁵We confirmed the findings of [159] and [160], that this approximation is accurate within a few percent in almost all scenarios.

format of the CP-conserving NMSSM.¹⁶ The resulting output is written to the NMSSM SLHA file provided by the user and takes the form

```
BLOCK RELICDENSITY # Relic density generated via freeze-out
  0 some number # DM Mass
  1 some number # Relic density
  2 some number # Likelihood
  3 some number # NOT ALLOWED
#
BLOCK DDETECTION # Direct Detection Crosssection of Proton, Neutron and Xenon
  0 some number # DM Mass
  1 some number # Proton DD-Crosssection
  2 some number # Neutron DD-Crosssection
  3 some number # Xenon DD-Crosssection
  4 some number # 2Sigma upper bound from LZ
  5 some number # Likelihood
  6 some number # NOT ALLOWED
#
```

Here, also the results of the likelihood functions are saved, which we will describe in Sec. 11.3.

¹⁶Future versions of the code will improve the input, such that only a single input file is needed.

In the previous chapters, we described in detail how the DM observables are obtained. This chapter provides an overview of the tool **NMSSMScanner**, the additional observables tested, and the computer codes used. Further, we will provide the ranges of our parameter scan.

11.1. Organization of the Scan

To perform our analysis, we use a modified version of the Python code **BSMArt** [161]. This code allows us to connect all relevant programs and pass the necessary information of a given BSM model through the program chain. In **BSMArt**, it is possible to use different scanning techniques, such as Active Learning [162], Markov-Chain Monte Carlo (MCMC), random scans, or user-defined algorithms to scan the parameter space. Since **BSMArt** was initially developed as a complementary framework to **SARAH/SPHeno** [163, 164], it has proven effective across many BSM frameworks [162, 165–173].

Higgs and SUSY Spectra and Decays

In order to calculate the Higgs and SUSY mass spectra, we link the Fortran code **NMSSMCALC** [174] to **BSMArt**. The code computes the SUSY mass spectrum at leading order and evaluates the Higgs boson mass spectrum in the CP-violating NMSSM (CNMSSM), including full one-loop corrections [175, 176] as well as important two-loop QCD and electroweak corrections of order $\mathcal{O}(\alpha_t \alpha_s)$ [177], $\mathcal{O}(\alpha_t^2)$ [178] and $\mathcal{O}((\alpha_t + \alpha_\lambda + \alpha_\kappa)^2)$ [179]. **NMSSMCALC** additionally provides predictions for the leptonic anomalous magnetic moments and the EDM at one- and two-loop level [180, 181]. Furthermore, **NMSSMCALC** computes the Higgs boson decay widths and branching ratios. These calculations have been adopted from the Fortran code **HDECAY**. Also, **NMSSMCALC** is used to calculate the SUSY particle decays, including tree-level two- and three-body decays, loop-induced decays, and NLO SUSY-QCD corrections for processes involving color-charged particles [182].

Single and di-Higgs Production

In order to comply with the single Higgs boson production constraints regarding the LHC SM-like Higgs boson data and the exclusion limits from BSM Higgs boson searches at the

LHC, LEP, and Tevatron, we link **BSM_{art}** with the public **C++** code **HiggsTools** [109]. Using the loop-corrected Higgs boson masses as well as the effective Higgs boson couplings obtained by **NMSSMCALC**, the code computes the single SM-like and the non-SM-like Higgs production cross section, which are then multiplied by the corresponding branching ratios. These are then tested against the current experimental constraints. To comply with the non-resonant di-Higgs searches, we validate our computed SM-like Higgs pair-production cross sections against the experimental limits. The ATLAS collaborations set an upper limit of 2.9 times the inclusive Higgs boson pair production cross sections from gluon fusion (ggF) and vector boson fusion (VBF), with [183]

$$\sigma_{\text{upper}}^{\text{VBF, ggF}} = 32.8_{-7.1}^{+2.1} \text{ fb} \quad \text{at 95\% CL.} \quad (11.1)$$

At the CMS collaboration, an upper limit of 3.4 times the SM expectation at 95% CL is set, such that it reads [184]

$$\sigma_{\text{upper}}^{\text{VBF, ggF}} = 32.76_{-6.83}^{+1.95} \text{ fb} \quad \text{at 95\% CL.} \quad (11.2)$$

To calculate the non-resonant di-Higgs production cross section, we use the Fortran code **HPair** [185].¹⁷ The resonant di-Higgs constraints are checked by **HiggsTools**. We multiply the production cross section of a non-SM-like single boson, which is obtained with the code **SusHi** [188–190], with their branching ratios into a SM-like Higgs boson pair. This quantity is then checked against the experimental measurements.

SUSY Searches

In our analysis, we use the code **SModelS** [191–194] to check the constraints from SUSY searches. **SModelS** computes the leading-order squark and gluino pair production cross section via **PYTHIA** [195]. Additionally, it applies a *K*-Factor for the QCD corrections from **NLL-Fast** [196–203] at next-to-leading logarithmic order matched to next-to-leading order. The electroweakino pair-production cross sections are obtained using an in-house code. Here, we apply for the NLO electroweak corrections an approximate *K*-factor of 1.3, which can be used when the electroweakinos are lighter than the squarks [204, 205]. At leading order, the mixed squark-electroweakino pair production is computed by **SModelS**. The total cross section of multi-particle final states in the SUSY scenario is then obtained by combining the production cross sections with the SUSY particle branching ratios obtained by **SDECAY** [206], which includes the SUSY particle decays in the NMSSM [182]. The total cross section is then compared with the experimental analyses.

DM Observables

As stated in the previous chapters 10 and 9, we compute the relic density and the direct-detection cross section of the lightest neutralino using **RelExt**, which was extended to include also the NMSSM as a model. The relic density is compared with the experimental limit given in Eq. (3.22). We use Eq. (9.37) to compare with the latest exclusion bounds of the **Lux-Zeplin** experiment [4].

Electroweak Precision Observables

We use the *W* boson mass prediction computed by **NMSSMCALC** to check for compatibility with the electroweak precision observables. The mass prediction is compared against the world average for the *W* boson mass, which reads [152]

$$M_W = 80.3692 \pm 0.0266 \pm 0.01 \text{ GeV} . \quad (11.3)$$

¹⁷Note that the non-resonant di-Higgs searches are not expected to constrain the NMSSM parameter space, cf. Refs. [186, 187]. Therefore, we will only check the constraints of the non-resonant di-Higgs production after obtaining the parameter sample.

11.2. Parameter Ranges

The SM input parameters are given by

$$\begin{aligned}
G_F &= 1.66370 \times 10^{-5} \text{ GeV}^{-2} & m_\mu &= 0.105658367 \text{ GeV} \\
\alpha_{\text{em}}^{-1}(M_Z) &= 127.995 & m_\tau &= 1.77682 \text{ GeV} \\
\alpha_S(M_Z) &= 0.1179 & \bar{m}_s^{\text{MS}}(2 \text{ GeV}) &= 0.95 \text{ GeV} \\
M_Z &= 91.1876 \text{ GeV} & \bar{m}_c^{\text{MS}}(\bar{m}_c^{\text{MS}}) &= 1.274 \text{ GeV} \\
M_W &= 80.3790 \text{ GeV} & \bar{m}_b^{\text{MS}}(\bar{m}_b^{\text{MS}}) &= 4.18 \text{ GeV} \\
&& m_t &= 172.76 \text{ GeV}.
\end{aligned}$$

In Tab. 11.1, we list the input parameters and their respective scan boundaries. Since we perform our analysis in the CP-conserving NMSSM, the input parameters are taken to be real. Following the conventions of the SUSY Les Houches Accord (SLHA) [207], we treat the soft SUSY-breaking mass parameters, trilinear couplings, the higgsino mass, and $\tan \beta$ as $\overline{\text{DR}}$ parameters evaluated at the scale μ_0

$$\mu_0 = M_{\text{SUSY}} = \sqrt{m_{\tilde{Q}_3} m_{\tilde{t}_R}}. \quad (11.4)$$

This scale is also used as the renormalization scale in the computation of the higher-order corrections. Note that the charged Higgs boson mass is taken as an input parameter, where the lower bound is given at 600 GeV, in order to comply with the type-II B physics constraints for a type II 2HDM-like scalar sector from $b \rightarrow s\gamma$ [208–213]. This constraint implies that all other doublet-like non-SM-Higgs bosons are rather heavy. To fulfill perturbativity, we impose the following rough constraint

$$\lambda^2 + \kappa^2 \leq 0.7. \quad (11.5)$$

In order to comply with the experimentally measured Higgs boson, we require that one of the neutral Higgs bosons behaves very SM-like and that the mass of this scalar boson H is in the range of

$$124 \text{ GeV} \leq m_H \leq 126 \text{ GeV}. \quad (11.6)$$

parameter	scan range [TeV]	parameter	scan range
$m_{H^\pm}$	[0.6, 4]	μ_{eff}	[0.1, 4] TeV
M_1, M_2	[0.1, 4]	$A_{t,b,\tau}$	[-4, 4] TeV
M_3	[0.4, 4]	A_κ	[-4, 0.1] TeV
$m_{\tilde{Q}_3}, m_{\tilde{t}_R}, m_{\tilde{b}_R}$	[0.4, 4]	$\tan \beta$	[1, 20]
$m_{\tilde{L}_3}, m_{\tilde{\tau}_R}$	[0.4, 4]	λ	[0.01, 1]
$m_{\tilde{Q}_2}, m_{\tilde{u}_R}$	[0.4, 4]	κ	[0.01, 1]

Table 11.1.: Ranges for the scan over the NMSSM parameter space. We set $m_{\tilde{L}_1} = m_{\tilde{L}_2} = m_{\tilde{Q}_1} = m_{\tilde{Q}_2}$ and $m_{\tilde{u}_R} = m_{\tilde{c}_R} = m_{\tilde{d}_R} = m_{\tilde{s}_R} = m_{\tilde{e}_R} = m_{\tilde{\mu}_R}$.

11.3. Scan Procedure

We generate a parameter sample using the tool **NMSSMScanner**, optimizing an MCMC scan with likelihood functions for each individual final state considered. This means that at first, we perform a random scan over the ranges provided in Tab. 11.1 and use these points as seeds for the MCMC scan. As a proof-of concept of the new tool **NMSSMScanner**, we try to obtain the maximum cross section values for the resonant production of a Higgs boson X , which subsequently decays into a SM-like plus non-SM-like Higgs boson pair $X \rightarrow HY$, we optimize the MCMC scan with likelihood functions $\mathcal{L}$. For example ¹⁸, for the maximization of the scalar resonance, we chose the following likelihood function

$$\mathcal{L}_{\max}^s = \exp\{(s_0(\sigma \times \text{BR})/\mu)\}, \quad (11.7)$$

where σ denotes the production cross section of HY and BR denotes the product of the branching ratio of H and Y decaying into the considered finale state. The normalization $\mu = \sigma_{\text{seed}} \times \text{BR}_{\text{seed}}$ is calculated at the seed point. In our analysis, we set $s_0 = 2$, as this was found to be the optimal value for convergence.

¹⁸For a more detailed overview of the procedure, we refer to Ref. [128]

In this chapter, we will present the results for the maximum cross sections obtained for the production of a pair consisting of a SM-like Higgs boson (H) and a non-SM-like Higgs boson (Y). These are produced by a resonant decay of the heavier Higgs boson (X), which has been produced via gluon fusion at a center-of-mass energy $\sqrt{s} = 13$ TeV. The production cross-section is then given by

$$\sigma_{HY}^{s/p} = \sigma(gg \rightarrow X) \times \text{BR}(X \rightarrow HY) , \quad (12.1)$$

where the superscripts s and p denote whether the heavier X is a scalar ($s \equiv h_3^0$) or a pseudoscalar ($p \equiv A_2$). Therefore, we have

$$\sigma_{HY}^s = \sigma(gg \rightarrow h_3^0) \times \text{BR}(h_3^0 \rightarrow h_1^0 h_2^0) , \quad (12.2)$$

$$\sigma_{HY}^p = \sigma(gg \rightarrow A_2) \times \text{BR}(A_2 \rightarrow h_{1/2}^0 A_1) . \quad (12.3)$$

Depending on the benchmark scenario, either h_1^0 or h_2^0 can be the SM-like Higgs boson. We will present the results for the following final states

$(b\bar{b})(b\bar{b})$ final state:	$\sigma_{HY}^{s/p} \times \text{BR}(H \rightarrow b\bar{b}) \times \text{BR}(Y \rightarrow b\bar{b})$	[214, 215]	
$(b\bar{b})(\tau\tau)$ final state :	$\sigma_{HY}^{s/p} \times \text{BR}(H \rightarrow \tau^+ \tau^-) \times \text{BR}(Y \rightarrow b\bar{b})$	[216]	
$(b\bar{b})(\gamma\gamma)$ final state :	$\sigma_{HY}^{s/p} \times \text{BR}(H \rightarrow \gamma\gamma) \times \text{BR}(Y \rightarrow b\bar{b})$	[217–219]	
	$\sigma_{HY}^{s/p} \times \text{BR}(H \rightarrow b\bar{b}) \times \text{BR}(Y \rightarrow \gamma\gamma)$	[220]	
$(\tau\tau)(\gamma\gamma)$ final state :	$\sigma_{HY}^{s/p} \times \text{BR}(H \rightarrow \gamma\gamma) \times \text{BR}(Y \rightarrow \tau\tau)$	[221]	(12.4)
	$\sigma_{HY}^{s/p} \times \text{BR}(H \rightarrow \tau\tau) \times \text{BR}(Y \rightarrow \gamma\gamma)$	[221]	
$(b\bar{b})(t\bar{t})$ final state :	$\sigma_{HY}^{s/p} \times \text{BR}(H \rightarrow b\bar{b}) \times \text{BR}(Y \rightarrow t\bar{t})$		
$(6b)$ final state from $(3H)$:	$\sigma_{HY}^s \times \text{BR}(Y \rightarrow HH) \times (\text{BR}(H \rightarrow b\bar{b}))^3$	[222, 223]	
$(\gamma\gamma)(WW)$ final state :	$\sigma_{HY}^s \times \text{BR}(H \rightarrow \gamma\gamma) \times \text{BR}(Y \rightarrow WW)$	[224]	.

Here, the citations refer to the ATLAS and CMS analyses, where the respective final states have been investigated.

Maximum Cross Section Values

In this section, we show the results for the benchmark scenarios presented in Ref. [128]. Here, we further extend these results to the DM observables, which we have implemented in the code `ReLExt` within the scope of this project. As an example of our methodology, we present the scan results of our tool for the $4b$ final state. The experimental results of this final state have been provided by the CMS collaboration in Ref. [214]. In Fig. 12.1, we present the cross section values of the production of a resonantly produced non-SM-like Higgs boson X into a $4b$ final state in the plane (m_X, m_Y) plane. The maximum cross section values are denoted by the color of the hexagonal bins, with the color bar showing the range of cross-section values in units of fb. For each hexagon, we group parameter points within a 50 GeV range in both m_X and m_Y , and select the parameter point with the largest production cross section. The choice is justified because the NMSSM masses are not input parameters but derived quantities. On the top (bottom) plot of Fig. 12.1, we show the production of a SM-like Higgs boson and a scalar (pseudoscalar) non-SM-like Higgs boson Y via an intermediate scalar non-SM-like Higgs boson X . The crosses in both plots mark the benchmark points that yield the maximum production cross-section in the $4b$ final state in the scanned parameter region. In a similar fashion, we search for the parameter space with the largest cross section in the various final states given in Eq. (12.4).

Furthermore, we provide in Tabs. 12.1 and 12.2 the maximum cross section values for the $4b$, the $(2b)(2\tau)$, the $(2b)(2\gamma)$, and the $(2\tau)(2\gamma)$ final states for resonantly produced scalar (Tab. 12.1) or a resonantly produced pseudoscalar intermediate state (Tab. 12.2). Additionally, we provide the name of the benchmark point and the tables that list the input parameters and relevant information on single- and di-Higgs cross sections.¹⁹ In Tab. 12.3, we list benchmark points where the non-SM-like Higgs boson decays into heavier final states, i.e., $t\bar{t}$, SM-like Higgs bosons HH and WW final states. Furthermore, compared to Ref. [128], we extend Tabs. 12.1, 12.2, and 12.3 by providing additional information on dark matter observables. These include the lightest neutralino mass $m_{\tilde{\chi}_1^0}$, the relic density Ωh^2 , the dominant annihilation channel contributing to the relic density calculation together with its percentage contribution, the spin-independent direct detection cross section $\sigma_{\text{SI-DD-N}}$, and the corresponding exclusion limit $\sigma_{\text{SI-DD,exp}}$ from the `LUX-Zeplin` experiment. The DM observables have been obtained by `ReLExt`. In all scenarios of the light final states, the charged and the neutral doublet-like non-SM-like Higgs bosons, the latter of which appear as the scalar resonance H_3 and the pseudoscalar resonance A_2 , are close in mass with around 600 GeV. Furthermore, the total widths are at most 20 GeV and the widths of the singlet-like and the SM-like Higgs boson are small compared to the its masses. Therefore, the narrow-width approximation used in this analysis is well motivated. In all of our benchmark points, the values of $\tan\beta$ are small, which is usual for NMSSM scenarios. The values of the NMSSM-specific parameters κ and λ are around 0.5. This due to the unitarity constraint given in Eq. (11.5). Due to the constraints on the SM-like Higgs boson mass, the soft-SUSY breaking stop parameter values range between -3 TeV and -4 TeV.

Dark Matter Observables

In our benchmark points, the lightest neutralino $\tilde{\chi}_0$, which is the dark matter candidate in the NMSSM, has masses in the range of 189 to 390 GeV. Furthermore, none of the presented benchmark points saturate the observed relic density. The benchmark points `Bp2b2gam`, `Bs2b2gam`, `Bps2b2t`, and `Bp2b2t`, where the intermediate state Y decays either into 2γ or $t\bar{t}$, the relic density is primarily determined by dark matter annihilation into $t\bar{t}$. The reasoning is clear in the 2γ case: As the decay of the scalar intermediate particles is loop-induced

¹⁹The input parameters of each benchmark point are given in App. C.

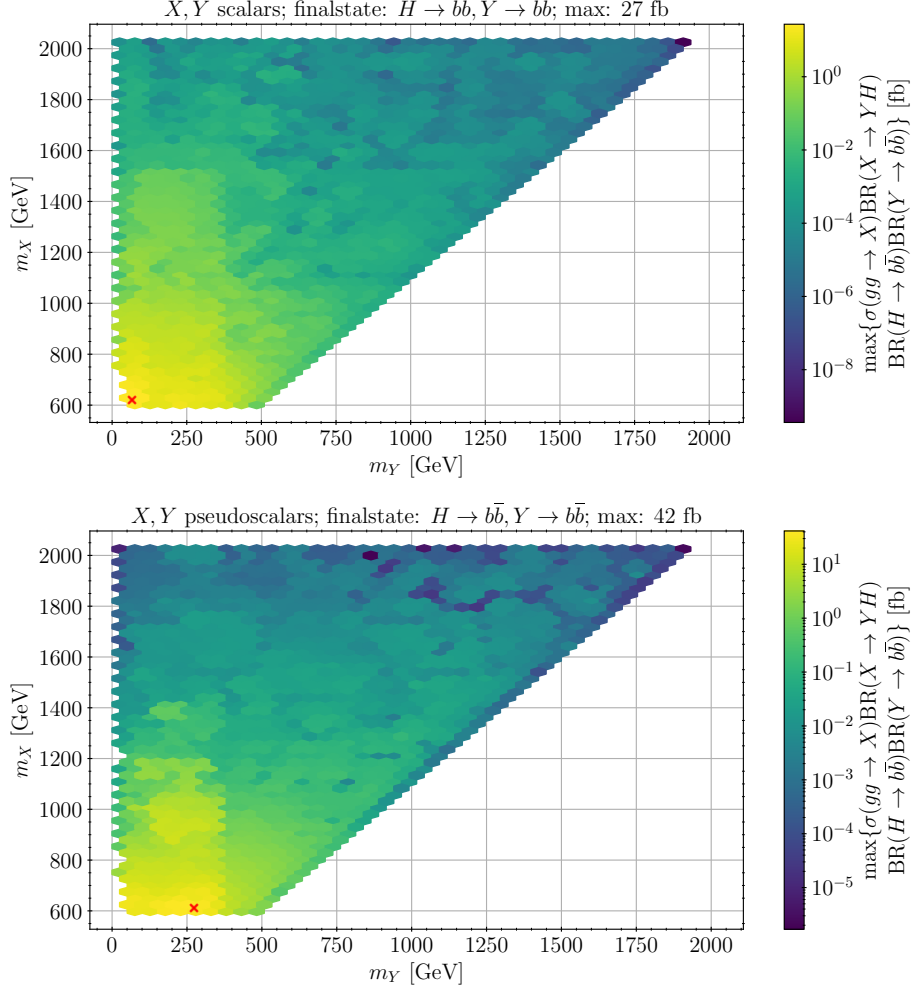


Figure 12.1.: The mass of the resonantly produced X , m_X , where $x = \text{scalar/pseudo scalar}$ in the top (bottom) plot as a function of m_Y . The maximal cross section for the resonant scalar (pseudoscalar) production of the SM-like and non-SM-like Higgs pair HY , followed by a decay into $H \rightarrow b\bar{b}$ and $Y \rightarrow b\bar{b}$ is denoted by the color gradient in the top (bottom) plot. The red crosses mark the benchmark point with the maximum cross-section value. Taken from [128].

through a top-quark loop, the Higgs- $t\bar{t}$ coupling is increased, as we are trying to maximize that final state. This same reasoning can also be applied in the case of a $t\bar{t}$ pair in the final state. In the benchmark points **BPs4b** and **BPs2gam2b**, the neutralino is higgsino-like and can efficiently annihilate into a gauge boson pair. In both scenarios, the dominant and second dominant annihilation channels are $\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow W^+ W^-$ and $\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow ZZ$, respectively. This is also consistent with the literature, cf. [49], where it is stated that if the neutralino is higgsino-like, it can efficiently annihilate into a gauge boson pair. In the benchmark points **BPs3H6b** and **BPs2gamma2w**, also here the neutralino is higgsino-like; however, the neutralino mass is high enough, i.e., $m_{\tilde{\chi}_1^0} > m_t$, to efficiently annihilate into a $t\bar{t}$ pair. This is also in compliance with the literature, cf. [49]. To understand why the annihilation into a $t\bar{t}$ pair is not the dominant channel in the benchmark points **BPs4b** and **BPs2gam2b**, where the neutralino mass is also larger than the top mass, we have to investigate the annihilation cross-section. The annihilation cross section into a $t\bar{t}$ pair is proportional to the kinematic factor $\beta_t = (1 - 4m_t^2/s)$. The important region of the integration in Eq. (9.30) is at the

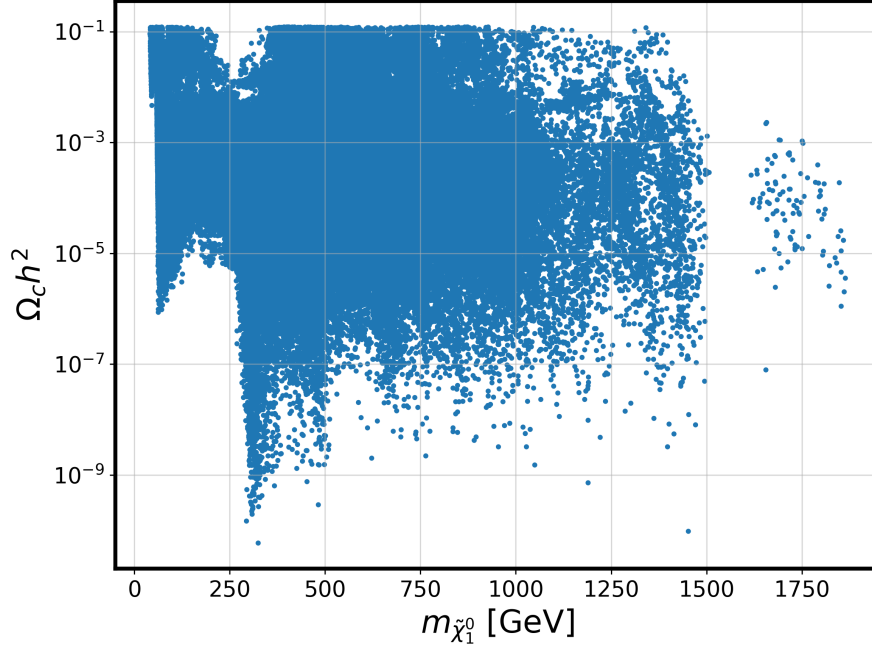


Figure 12.2.: The computed relic density $\Omega_c h^2$ as a function of the neutralino mass $m_{\tilde{\chi}_1^0}$ for the scanned parameter sample.

lower bound, as the upper limit is Boltzmann suppressed. Therefore, the value of s can be taken at $4m_{\tilde{\chi}_1^0}^2 + \epsilon$, where ϵ is a small positive number. In these benchmark scenarios BPs4b and BPs2gam2b, the neutralino mass $m_{\tilde{\chi}_1^0} \approx 200$ GeV, which means the kinematic factor is approximately $\beta_t \sim 0.51$, which suppresses the annihilation into a $t\bar{t}$ pair. However, in the benchmark points BPs3H6b and BPs2gamma2w the neutralino mass is larger at around 300 GeV, which leads to a kinematic factor of ~ 0.81 , which leads to the efficient annihilation into a $t\bar{t}$ pair. In the benchmark point BPp4b, the dominant channel contributing to the relic abundance is the light pseudoscalar pair $A_1 A_1$ final state. This is understood by investigating the scalar masses of this parameter point. Here, as the light pseudoscalar mass m_{A_1} is smaller than the neutralino mass $m_{\tilde{\chi}_1^0}$, we start the integration over s in the TAC given in Eq. (9.30) at $s = 4m_{\tilde{\chi}_1^0}^2$. Note that we are integrating over the resonance of the heavy neutral Higgs boson, which enhances the annihilation cross section and therefore the thermal average cross section, thereby decreasing the relic density.

Next, we want to investigate whether it is possible to saturate the relic density while still complying with direct-detection constraints. In Fig. 12.2, we show the computed relic density $\Omega_c h^2$ as a function of the neutralino mass $m_{\tilde{\chi}_1^0}$ for the full scan sample. It can be seen, that the full dark matter relic density can be obtained, with parameter points, that fulfill all relevant experimental and theoretical constraints, up to a DM mass of ~ 1.4 TeV.²⁰ In Fig. 12.3, we present the SI-DD-N cross section $\sigma_{\text{SI-DD-N}}$ as a function of the neutralino mass $m_{\tilde{\chi}_1^0}$. The color bar indicates the computed ratio of the computed relic density $\Omega_c h^2$ and the experimental measured value given in Eq. (3.22). All shown points fulfill all relevant experimental and theoretical constraints. The conclusion is that it is possible to find parameter points that comply with the measurement of the Lux-Zeplin collaboration, saturate the full relic density, and lie above the neutrino floor [225], which lies below 10^{-11} and 10^{-12} fb, in the shown

²⁰Note that in the mass range between 170 and 350 GeV, no parameter points have been found in our current scan. We expect this to be a scan artifact and can investigate it in future work.

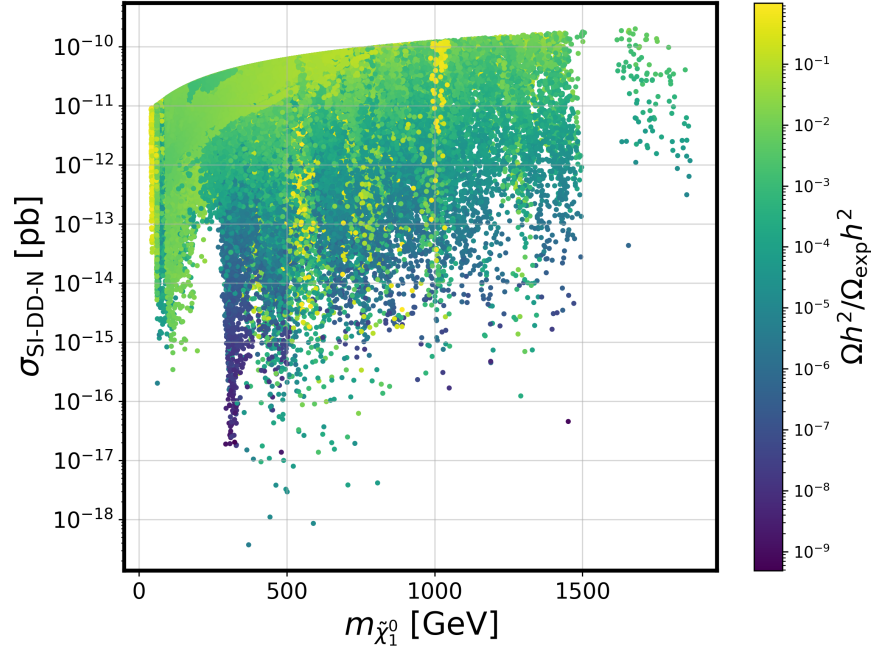


Figure 12.3.: $\sigma_{\text{SI-DD-N}}$ as a function of the DM mass $m_{\tilde{\chi}_1^0}$. The color gradient shows the computed relic density $\Omega_c h^2$.

mass ranges. Therefore, it is possible to test these parameter points in future DM-nucleon scattering experiments.

BP name	BPs4b, Tabs. C.1, C.2	BPs2b2gam Tabs. C.3, C.4	BPs2gam2b, Tabs. C.5, C.6
final state	$(H \rightarrow b\bar{b})(Y \rightarrow b\bar{b})$	$(H \rightarrow b\bar{b})(Y \rightarrow \gamma\gamma)$	$(H \rightarrow \gamma\gamma)(Y \rightarrow b\bar{b})$
$\sigma_{\max}^s$ [fb]	27	0.119	0.121
final state	$(H \rightarrow \tau\bar{\tau})(Y \rightarrow b\bar{b})$	$(H \rightarrow \tau\bar{\tau})(Y \rightarrow \gamma\gamma)$	$(H \rightarrow \gamma\gamma)(Y \rightarrow \tau\bar{\tau})$
$\sigma_{\max}^s$ [fb]	2.9	0.013	0.012
$m_{\tilde{\chi}_1^0}$ [GeV]	189.807	290.810	203.875
$\Omega_c h^2$	3.17×10^{-3}	1.295×10^{-4}	2.538×10^{-3}
Dominant Channel	$\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow W^+ W^-$ (32.5%)	$\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow t\bar{t}$ (83.83%)	$\tilde{\chi}_1^0 \rightarrow W^+ W^-$ (30.91%)
$\sigma_{\text{SI-DD,exp}}$ [pb]	2.4541×10^{-11}	3.6429×10^{-11}	2.6190×10^{-11}
$\sigma_{\text{SI-DD-N}}$ [pb]	1.4565×10^{-11}	2.419×10^{-11}	5.56×10^{-13}

Table 12.1.: Benchmark points with the maximum cross-section values for the resonant scalar production $X \equiv H_3$, followed by the decay into a SM-like Higgs boson H and a non-SM-like scalar Higgs boson $Y = H_1$ or H_2 in the $4b$, the $(2b)(2\tau)$, the $(2b)(2\gamma)$, and the $(2\tau)(2\gamma)$ final states. In addition, the DM mass $m_{\tilde{\chi}_0}$, the relic density $\Omega_c h^2$, the dominant channel in the relic abundance calculation together with its percentage contribution, the experimental direct detection cross-section limit at the DM mass, $\sigma_{\text{SI-DD,exp}}$, and the calculated direct-detection cross section $\sigma_{\text{SI-DD-N}}$ are provided. References to the corresponding tables containing the complete benchmark information are also provided. Taken from Ref. [128]

BP name	BPp4b, Tabs. C.7, C.8	BPp2b2gam Tabs. C.9, C.10
final state	$(H \rightarrow b\bar{b})(Y \rightarrow b\bar{b})$	
$\sigma_{\max}^p$ [fb]	42	
final state	$(H \rightarrow \tau\tau)(Y \rightarrow b\bar{b})$	
$\sigma_{\max}^p$ [fb]	4.5	
final state	$(H \rightarrow \gamma\gamma)(Y \rightarrow b\bar{b})$	$(H \rightarrow b\bar{b})(Y \rightarrow \gamma\gamma)$
$\sigma_{\max}^p$ [fb]	0.16	0.35
final state	$(H \rightarrow \gamma\gamma)(Y \rightarrow \tau\tau)$	$(H \rightarrow \tau\tau)(Y \rightarrow \gamma\gamma)$
$\sigma_{\max}^p$ [fb]	0.02	0.038
$m_{\tilde{\chi}_1^0}$ [GeV]	334.938	305.377
$\Omega_c h^2$	9.802×10^{-4}	3.1027×10^{-4}
Dominant Channel	$\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow A_1 A_1$ (63.6%)	$\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow t\bar{t}$ (89.95%)
$\sigma_{\text{SI-DD,exp}}$ [pb]	4.1644×10^{-11}	3.8149×10^{-11}
$\sigma_{\text{SI-DD-N}}$ [pb]	3.7899×10^{-11}	3.7125×10^{-11}

Table 12.2.: Benchmark points with the largest production cross sections for the resonant pseudoscalar production $X \equiv A_2$, followed by the decay $A_2 \rightarrow HA_1$, are shown for the $4b$, $(2b)(2\tau)$, $(2b)(2\gamma)$, and $(2\tau)(2\gamma)$ final states. In addition, the DM mass $m_{\tilde{\chi}_1^0}$, the relic density $\Omega_c h^2$, the dominant channel in the relic abundance calculation together with its percentage contribution, the experimental direct-detection cross section limit at the DM mass, $\sigma_{\text{SI-DD,exp}}$, and the calculated direct detection cross-section $\sigma_{\text{SI-DD-N}}$ are provided. References to the corresponding tables containing the complete benchmark information are also provided. Taken from Ref. [128].

BP name	BPs2b2t, Tabs. C.11, C.12	BPp2b2t Tabs. C.13, C.14
final state	$(H \rightarrow b\bar{b})(Y \rightarrow t\bar{t})$	$(H \rightarrow b\bar{b})(Y \rightarrow t\bar{t})$
$\sigma_{\max}^{s/p}$ [fb]	30	37
$m_{\tilde{\chi}_1^0}$ [GeV]	422.54	310.321
$\Omega_c h^2$	3.813×10^{-4}	1.1426×10^{-4}
Dominant channel	$\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow t\bar{t}$ (89.56%)	$\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow t\bar{t}$ (76.97%)
$\sigma_{\text{SI-DD,exp}}$ [pb]	5.2014×10^{-11}	3.8733×10^{-11}
$\sigma_{\text{SI-DD-N}}$ [pb]	1.2065×10^{-11}	3.8362×10^{-11}
BP name	BPs3H6b, Tabs. C.15, C.16	BPs2gamma2w Tabs. C.17, C.18
final state	$(H \rightarrow b\bar{b})(Y \rightarrow HH \rightarrow 4b)$	$(H \rightarrow \gamma\gamma)(Y \rightarrow WW)$
$\sigma_{\max}^s$ [fb]	4.03	0.104
$m_{\tilde{\chi}_1^0}$ [GeV]	292.671	296.970
$\Omega_c h^2$	6.3961×10^{-5}	4.8751×10^{-5}
Dominant channel	$\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow t\bar{t}$ (85.94%)	$\tilde{\chi}_1^0 \tilde{\chi}_1^0 \rightarrow t\bar{t}$ (88.21%)
$\sigma_{\text{SI-DD,exp}}$ [pb]	3.66×10^{-11}	3.7157×10^{-11}
$\sigma_{\text{SI-DD-N}}$ [pb]	2.822×10^{-11}	1.4737×10^{-11}

Table 12.3.: Benchmark points with the maximum cross-section values into heavier final states: Top row: resonant scalar H_3 (left) and pseudoscalar A_2 (right) production of HY , which decays decaying into $(b\bar{b})(t\bar{t})$ final states. Bottom row: Resonant scalar H_3 production of HY , followed by the decays into $(H \rightarrow b\bar{b})(Y \rightarrow HH \rightarrow 4b)$ (left) and into $(\gamma\gamma)(WW)$ (right). In addition, the DM mass $m_{\tilde{\chi}_0}$, the relic density $\Omega_c h^2$, the dominant channel in the relic abundance calculation together with its percentage contribution, the experimental direct-detection cross section limit at the DM mass, $\sigma_{\text{SI-DD,exp}}$, and the calculated direct detection cross-section $\sigma_{\text{SI-DD-N}}$ are provided. Taken from Ref. [128].

CHAPTER 13

Conclusion

In this part of the thesis, we presented the program package **NMSSMScanner**, which is built to efficiently scan the complex parameter space of the NMSSM. Within the scope of this project, we implemented the NMSSM relic density and the direct-detection cross section calculation in the public code **ReLExT**. We have presented the necessary framework for calculating the relic density and the direct-detection cross section in the NMSSM. Afterward, we gave an overview of the public code **ReLExT** in Ch. 10 and described how we automate the implementation of an arbitrary model in **ReLExT**. In Ch. 11, we presented how we organize the program chain in the program package **NMSSMScanner**. Here, we discuss the various experimental constraints included in our analysis. In Chapter 12, we presented as a proof of concept benchmark points, which maximize the cross section of a SM-like and non-SM-like Higgs boson pair, which is produced by a resonant scalar or pseudoscalar Higgs boson, in various decay channels. Further, we extended the investigation compared to Ref. [128] by providing, for each benchmark point, information on the DM observables, i.e., the DM relic density and the direct-detection cross section. Also, we investigated the possibility of obtaining the correct relic density in the NMSSM while still complying with the exclusion limit of **LUX-Zeplin**. We have shown that there is still a parameter region that saturates the relic density, complies with the exclusion limits of the **Lux-Zeplin** collaboration, and lies above the neutrino floor. In summary, we provided a proof of concept for our new package **NMSSMScanner** and the extension of **ReLExT**, which can serve as a starting point for future investigations of the allowed parameter space and DM observables of the NMSSM.

Part IV.

**The Dark Matter Relic Density at
Next-to-Leading Order**

The SM has unsolved problems, one of which is the nature of dark matter. As described in Ch. 3, it is possible to extract from the CMB the current energy budget of dark matter in the universe. The dark matter relic abundance has been measured by the PLANCK collaboration to be $\Omega_c h^2 = 0.1200 \pm 0.0012$ [3]. This value acts as a constraining factor on the parameter space of models with dark matter candidates. Calculating the relic abundance from a theoretical point of view, for any model, involves computing the (co-)annihilation cross sections of dark matter into SM particles. In practice, this calculation is generally done at leading-order. However, as experiments become more and more precise, theoretical predictions also need to be precise. In Refs. [226–229], the electroweak next-to-leading order effects on the relic density have been investigated in the framework of the inert-doublet 2HDM. In this work we computed the full electroweak and QCD higher-order effects in the framework of the CxSM, described in Sec. 2.2. As described in Ch. 10, it is possible to choose between a variety of codes to calculate the relic abundance at leading-order for an arbitrary model. However, at next-to-leading order, this calculation becomes more difficult. In `MicrOMEGAs` [141,142,144,145] it is possible to include next-to-leading order corrections via predefined functions. Furthermore, the code `DM@NLO` [230] provides the next-to-leading order (SUSY) QCD corrections for dark matter (co-)annihilation in the Minimal Supersymmetric Standard Model. In this work, we use our code `RelExt`, which we introduced in Ch. 10, and extended the already implemented relic density at leading-order in the context of the CxSM by the calculation of next-to-leading order electroweak and QCD corrections to the annihilation cross section of a dark matter pair into SM particles. This work will serve as an initial example of the implementation of next-to-leading order corrections in `RelExt` for a specific model, as the goal is to later extend the code in such a way to allow for an easy implementation of next-to-leading order corrections in `RelExt` for arbitrary models.

We will present this work as follows. We outline the general idea of the next-to-leading order calculation in Sec. 14.1. As ultraviolet and infrared divergences can arise at next-to-leading order calculations, we have to cure these with an appropriate regularisation and renormalization scheme. We provide an overview of the used renormalization schemes in the CxSM and describe how we treat infrared divergences in our processes in Ch. 15. Furthermore, we present in Ch. 16 the applied theoretical and experimental constraints and also the scan ranges of our example parameter sample. In Ch. 17, we show our obtained results.

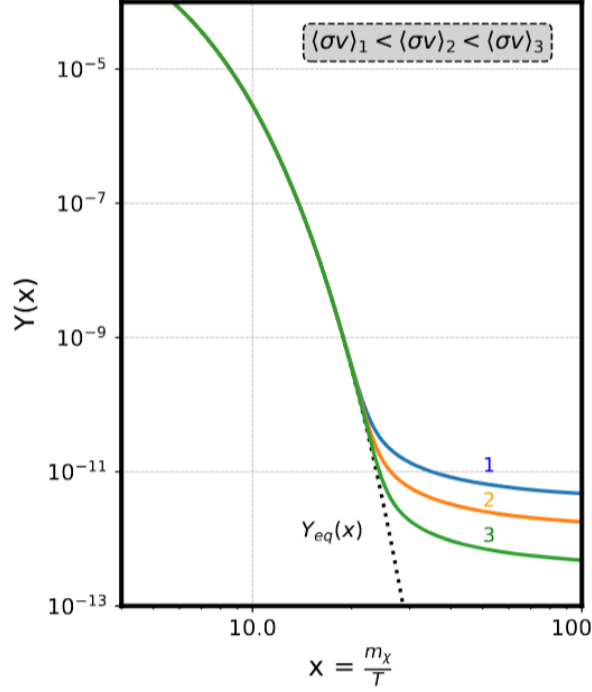


Figure 14.1.: Yield $Y(x)$ as a function of $x = \frac{m_\chi}{T}$, where m_χ denotes the mass of the dark matter particle. The dotted line denotes the equilibrium yield $Y_{\text{eq}}(x)$, while the colored lines denote the yield evolution for different values of the thermally averaged cross sections $\langle\sigma v\rangle_i$ ($i \in [1, 2, 3]$). Taken from Ref. [231].

14.1. Relic Density at Next-to-Leading Order

In Sec. 3.5, we derived the expressions to calculate the dark matter relic abundance, which is given by Eq. (3.69). This relic abundance is dependent on the thermally averaged cross section $\langle\sigma v\rangle$, which we derived in Sec. (9.1.1) and which is given by

$$\langle\sigma v\rangle = \frac{\sum_{i,j=1}^N g_i g_j \int_{(m_i+m_j)^2}^{\infty} ds \sqrt{s} p_{ij}^2 \sigma_{ij}(s) K_1\left(\frac{\sqrt{s}x}{m_\chi}\right)}{2T \left(\sum_{i=1}^N g_i m_i^2 K_2\left(\frac{m_i}{m_\chi}x\right)\right)^2}. \quad (14.1)$$

The influence of the thermally averaged cross section on the yield evolution, and hence via Eq. (3.69) on the relic abundance, can be seen in Fig. 14.1. Here, we schematically show the yield evolution as a function of $x = m_\chi/T$, where m_χ denotes the mass of the dark matter particle, for different values of the thermally averaged cross sections. It can be seen that for increasing cross sections the yield and hence the relic density decrease. The thermally averaged cross section is dependent on the $2 \rightarrow 2$ annihilation cross section σ_{ij} of a dark matter pair i, j into a all possible final state pairs (k, l) , which is given by

$$\sigma_{ij}^{\text{LO}} = \frac{1}{32\pi s g_i g_j} \sum_{k,l} \frac{\lambda^{1/2}(s, m_k^2, m_l^2)}{\lambda^{1/2}(s, m_i^2, m_j^2)} \int |\mathcal{M}_{ii \rightarrow kl}^{\text{LO}}|^2 d\cos\theta. \quad (14.2)$$

Here, $\mathcal{M}_{ii \rightarrow kl}^{\text{LO}}$ denotes the leading-order annihilation amplitude, λ is the Källén function, and θ is the azimuthal scattering angle. In the CxSM, there is only one dark matter candidate, hence, $i = j$. As we want to include the electroweak and QCD corrections in the thermally averaged cross section, we need to compute the next-to-leading order annihilation cross sec-

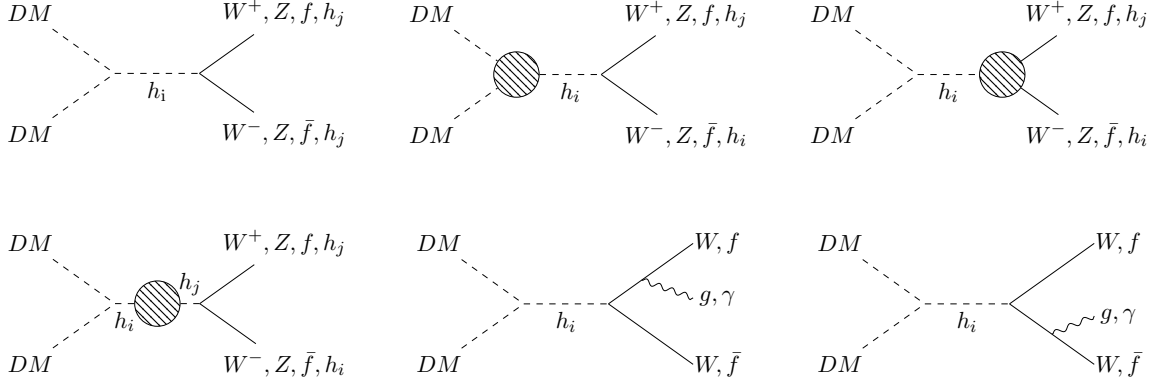


Figure 14.2.: Generic diagrams for DM annihilation into a massive gauge boson pair W^+W^- and ZZ , massive fermions f ($f \in [\tau, b, t]$) and a scalar pair $h_i h_j$ ($i, j \in [1, 2]$), respectively. Upper: leading-order contribution (left) and virtual vertex corrections (middle, right). Lower: self-energy corrections (left) and real radiation of massless photons and gluons (middle, right). The shaded blobs denote all possible loop and counterterm insertions in the CxSM.

tions. These are obtained by replacing the leading-order amplitudes with the next-to-leading order ones, $\mathcal{M}_{ij \rightarrow kl}^{\text{NLO}}$, in Eq. (14.2). The next-to-leading order squared amplitude is given by

$$|\mathcal{M}_{ij \rightarrow kl}^{\text{NLO}}|^2 = |\mathcal{M}_{ij \rightarrow kl}^{\text{LO}}|^2 + 2\text{Re}(\mathcal{M}_{ij \rightarrow kl}^{\text{LO}*}(\mathcal{M}_{ij \rightarrow kl}^{\text{VC}} + \mathcal{M}_{ij \rightarrow kl}^{\text{CT}})) , \quad (14.3)$$

where $\mathcal{M}_{ii \rightarrow kl}^{\text{VC}}$ and $\mathcal{M}_{ii \rightarrow kl}^{\text{CT}}$ are the amplitudes of the virtual corrections and the counterterms, respectively. If next-to-leading order amplitudes carry infrared divergences, we include the real corrections from $2 \rightarrow 3$ processes. We will provide an overview of how we deal with these kinds of divergences in Ch. 15. In Fig. 14.2, we show the generic diagrams of the leading and next-to-leading order annihilation processes into the final states provided in Tab. 14.1. Note that we do not consider light fermions, i.e., the first and second generation fermions, in our calculation. The reason is that at leading-order these channels contribute only a negligible amount to the total relic density. Therefore, we decided to omit these contributions in our analysis. In the next chapter, we will show how we obtain ultraviolet- and infrared-convergent next-to-leading order amplitudes in our work.

Initial state	Final state
AA	$h_i h_j$ ($i, j \in [1, 2]$), $W^- W^+$, ZZ ,
	$t\bar{t}$, $b\bar{b}$, $\tau\bar{\tau}$

Table 14.1.: Considered final states for the DM annihilation in the computation of the relic abundance.

Renormalization and the Treatment of Infrared Divergences in the CxSM

In higher-order calculations, ultraviolet (UV) and infrared (IR) divergences may arise. These must be handled appropriately to obtain physically meaningful and interpretable results. Ultraviolet divergences are handled by regularization and renormalization schemes. To cure the IR divergences, a different approach is used; see Sec. 15.5.

Dimensional regularization is a commonly used regularization method. In this approach, the loop integrals appearing in the calculation are evaluated in $D = 4 - 2\epsilon$ dimensions. The divergences then manifest as poles of inverse powers of ϵ (ϵ^{-1} for UV divergences and ϵ^{-1} and ϵ^{-2} for IR divergences). To render the physical amplitudes for a calculated process free of the UV poles, the input parameters must be redefined. The renormalized parameter κ and the corresponding counterterm $\delta\kappa$ are introduced such that the bare parameter κ_0 , which emerges in the unrenormalized Lagrangian $\mathcal{L}_0$, is defined as

$$\kappa_0 = \kappa + \delta\kappa \quad . \quad (15.1)$$

Furthermore, the bare fields ψ_0 are defined by a shift of the wave-function renormalization constant Z_ψ such that

$$\psi_0 = \sqrt{Z_\psi} \psi \approx \left(1 + \frac{\delta Z_\psi}{2}\right) \psi \quad . \quad (15.2)$$

The last term in Eq. (15.2) is obtained by expanding up to next-to-leading order. The counterterm $\delta\kappa$ and the wave-function renormalization constants (WFRC) δZ_ψ are determined by suitable renormalization conditions. The divergent parts of the counterterms cancel the UV divergences in the loop diagrams. In addition, finite terms arise, which are fixed by the renormalization conditions. For a more comprehensive description of renormalization, we refer to Refs. [5, 14, 232, 233].

In the next sections, we introduce the renormalization of the CxSM, following the descriptions in Refs. [25, 182, 234]. For different BSM theories, similar approaches have been used, cf. Ref [9] .

15.1. On-Shell Renormalization

The renormalization conditions for the mass parameters and the WFRs are fixed by the on-shell (OS) renormalization scheme [232]. Here, the renormalized self-energy $\hat{\Sigma}_\psi(p^2)$ of the field ψ is given as

$$\hat{\Sigma}_\psi(p^2) = \Sigma_\psi(p^2) - \delta m^2 + \delta Z_\psi(p^2 - m^2). \quad (15.3)$$

Here, $\Sigma_\psi(p^2)$ denotes the sum of all truncated and unrenormalized self-energy diagrams, and δm^2 and δZ_ψ denote the mass counterterm and the WFR for the field ψ , respectively. The first OS renormalization condition states that the propagator has a pole at the momentum squared corresponding to the physical mass squared, $p^2 = m^2$, requiring for the renormalized self-energy that

$$\hat{\Sigma}_\psi(m^2) = 0. \quad (15.4)$$

As the third term of Eq. (15.3) trivially vanishes for $p^2 = m^2$, the counterterm δm is then given by

$$\delta m = \Sigma_\psi(m^2). \quad (15.5)$$

To obtain an expression for the WFR, the second OS renormalization condition states that the residue of the propagator needs to be at the imaginary unit i . To fulfill this condition, the WFR must then be given by

$$\delta Z_\psi = - \left. \frac{\partial \Sigma_\psi(p^2)}{\partial p^2} \right|_{p^2=m^2}. \quad (15.6)$$

In BSM theories, mixing between fields can occur. Therefore, at next-to-leading order, one needs to define the renormalization conditions also for the non-diagonal components. This leads to the third OS renormalization condition, which states that at the poles of the i -th particle, $p^2 = m_i^2$, no mixing between the fields is allowed. Using Eq. (15.3), we obtain for mixing particles the following equation

$$\Sigma_{\psi_i \psi_j}(p^2) - \delta m_{ij} + \frac{\delta Z_{ij}}{2}(p^2 - m_i^2) + \frac{\delta Z_{ji}}{2}(p^2 - m_j^2) = 0; \quad i \neq j, \quad (15.7)$$

where δm_{ij} denotes the non-diagonal components of the mass-squared counterterm matrix, δZ_{ij} are the non-diagonal WFRs, and $\Sigma_{\psi_i \psi_j}$ is the unrenormalized self-energy with ψ_i in the initial state and ψ_j in the final state. From Eq. (15.7), we obtain $n(n-1)$ equations, where n is the number of mixing fields. These equations can now be solved for the non-diagonal WFRs. This leads to the following form

$$\delta Z_{ij} = \frac{2}{m_i^2 - m_j^2} \Sigma_{\psi_i \psi_j}(m_j^2), \quad i \neq j. \quad (15.8)$$

15.2. Scalar Sector

In the following, we describe the renormalization of the scalar sector of the CxSM, i.e., the mass and wave function renormalization, and the renormalization schemes of the singlet VEV v_s , the electroweak VEV v , and the mixing angle α .

Mass and Wave Function Renormalization

As mentioned earlier, we define the bare mass and bare fields as described in Eqs. (15.1) and (15.2), respectively. This leads for the pseudoscalar field A to the following relations

$$A_0 = \sqrt{Z_A} A \approx \left(1 + \frac{\delta Z_A}{2} \right) A, \quad (15.9)$$

$$m_{A,0}^2 = m_A^2 + \delta m_A^2. \quad (15.10)$$

For the scalar mass eigenstates h_1 and h_2 , the renormalization of the fields and the diagonalized mass matrix $D_{hh,0}^2$ is given by

$$\begin{pmatrix} h_{1,0} \\ h_{2,0} \end{pmatrix} = \sqrt{Z_{hh}} \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \approx \left(\mathbb{1} + \frac{\delta Z_{hh}}{2} \right) \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}, \quad (15.11)$$

$$D_{hh,0}^2 = D_{hh}^2 + \delta D_{hh}^2. \quad (15.12)$$

The counterterm matrices δZ_{hh} and δD_{hh}^2 have the following form

$$\delta Z_{hh} = \begin{pmatrix} \delta Z_{h_1 h_1} & \delta Z_{h_1 h_2} \\ \delta Z_{h_2 h_1} & \delta Z_{h_2 h_2} \end{pmatrix}, \quad \delta D_{hh}^2 = \begin{pmatrix} \delta D_{h_1 h_1}^2 & \delta D_{h_1 h_2}^2 \\ \delta D_{h_2 h_1}^2 & \delta D_{h_2 h_2}^2 \end{pmatrix}. \quad (15.13)$$

Furthermore, the tadpole counterterms δT_i ($i \in [1, 2]$) for the tadpoles T_i are defined as

$$\hat{T}_i = T_i - \delta T_i = 0, \quad (15.14)$$

where $\hat{T}_i$ are the vanishing renormalized tadpoles. For the tadpole renormalization, we use the Fleischer-Jegerlehner scheme [235]. In this renormalization description, an additional shift in the VEVs is added. With this shift, the tadpole contributions are included in the self-energies and, consequently, in the counterterms, as well as in the vertex corrections.²¹ In the following, we will label self-energy contributions with tadpole inclusions as Σ^{Tad} . The explicit results for the counterterms in terms of the momentum p and the masses are then given by

$$\begin{aligned} \delta m^2 &= \text{Re} \left(\Sigma_A^{\text{Tad}}(m_A^2) \right), \\ \delta Z_A &= -\text{Re} \left(\frac{\partial \Sigma_A^{\text{Tad}}(p^2)}{\partial p^2} \Big|_{p^2=m_A^2} \right), \\ \delta m_{h_i}^2 &= \text{Re} \left(\Sigma_{h_i h_i}^{\text{Tad}}(m_{h_i}^2) \right), \\ \delta Z_{h_i h_i} &= -\text{Re} \left(\frac{\partial \Sigma_{h_i h_i}^{\text{Tad}}(p^2)}{\partial p^2} \Big|_{p^2=m_{h_i}^2} \right), \\ \delta Z_{h_i h_j} &= \frac{2}{m_{h_i}^2 - m_{h_j}^2} \text{Re} \left(\Sigma_{h_i h_j}^{\text{Tad}}(m_{h_j}^2) \right). \end{aligned} \quad (15.16)$$

Renormalization of the Electroweak VEV v

The bare VEV v_0 is

$$v_0 = v + \delta v. \quad (15.17)$$

In order to fix the counterterm δv , we write v in terms of the SM parameters, which reads

$$v = \frac{2m_W \sqrt{m_Z^2 - m_W^2}}{em_Z}, \quad (15.18)$$

where m_W and m_Z are the masses of the $W^\pm$ and Z boson, respectively, and e is the electric charge. The VEV counterterm δv can then be written in terms of δm_W , δm_Z and δe , which are the counterterms of the respective parameters, such that we have

²¹For a more detailed description, we refer to Refs. [9, 236]

$$\delta v = v \left[\frac{1}{2(m_Z^2 - m_W^2)} \left(\frac{m_Z^2}{m_W^2} \delta m_W^2 - \frac{m_W^2}{m_Z^2} \delta m_Z^2 \right) + \delta Z_e \right]. \quad (15.19)$$

Here, we used $\delta e = e\delta Z_e$. We will provide the explicit expression for the counterterms in Sec. 15.3.

Renormalization of the Mixing Angle α

In this section, we will briefly show how the mixing angle α is renormalized. Analogous to the mass parameters, the mixing angle is split up as follows

$$\alpha_0 = \alpha + \delta\alpha, \quad (15.20)$$

where α_0 is the bare parameter, $\delta\alpha$ is the counterterm and α is the renormalized parameter. Even though there are other techniques, such as the $\overline{\text{MS}}$ scheme [5] or the process-dependent scheme [9], we will use the KOSY scheme [237] combined with the pinched scheme in this work. To derive the renormalization constant for the mixing angle in the KOSY scheme, we start by inserting Eq. (15.20) into the rotation matrix R_α given in Eq. (2.35). This leads to the following relation

$$R(\alpha + \delta\alpha) = \begin{pmatrix} \cos(\alpha + \delta\alpha) & \sin(\alpha + \delta\alpha) \\ -\sin(\alpha + \delta\alpha) & \cos(\alpha + \delta\alpha) \end{pmatrix} \approx \underbrace{\begin{pmatrix} 1 & \delta\alpha \\ -\delta\alpha & 1 \end{pmatrix}}_{R(\delta\alpha)} \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{pmatrix}. \quad (15.21)$$

The WFRs for the mass eigenstates can be written by

$$\begin{pmatrix} h_{1,0} \\ h_{2,0} \end{pmatrix} = R(\alpha_0) \begin{pmatrix} H_0 \\ S_0 \end{pmatrix} = R(\alpha + \delta\alpha) \sqrt{Z_\Phi} \begin{pmatrix} H \\ S \end{pmatrix}. \quad (15.22)$$

Here, $\sqrt{Z_\Phi}$ denotes the WFR matrix of the gauge eigenstates. We can rewrite Eq. (15.22) by inserting $\mathbb{1}_{2 \times 2} = R^T(\alpha)R(\alpha)$, which leads to

$$\begin{pmatrix} h_{1,0} \\ h_{2,0} \end{pmatrix} = R(\alpha + \delta\alpha) \sqrt{Z_\Phi} R^T(\alpha) R(\alpha) \begin{pmatrix} H \\ S \end{pmatrix} = \sqrt{Z_h} \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}, \quad (15.23)$$

where we defined the WFR matrix $\sqrt{Z_h}$ of the mass eigenstates as follows

$$\sqrt{Z_h} \equiv R(\delta\alpha) R(\alpha) \sqrt{Z_\Phi} R(\alpha)^T \approx \begin{pmatrix} 1 + \frac{\delta Z_{h_1 h_1}}{2} & \delta C + \delta\alpha \\ \delta C - \delta\alpha & 1 + \frac{\delta Z_{h_2 h_2}}{2} \end{pmatrix}. \quad (15.24)$$

Here, δC represents an auxiliary parameter. Since its explicit form is not needed for the subsequent discussion, we will not present its explicit form here. Since we use OS renormalization for the WFRs, the elements of $\sqrt{Z_h}$ are given as in Eq. (15.13). Therefore we can relate the off-diagonal elements of Eq. (15.13) to the ones of Eq. (15.24) and obtain two equations

$$\delta C + \delta\alpha = \frac{1}{2} \delta Z_{h_1 h_2}, \quad (15.25)$$

$$\delta C - \delta\alpha = \frac{1}{2} \delta Z_{h_2 h_1}, \quad (15.26)$$

which lead to the following expression for the renormalization constant of the mixing angle α ,

$$\delta\alpha = \frac{\delta Z_{h_1 h_2} - \delta Z_{h_1 h_2}}{4}. \quad (15.27)$$

In order to obtain gauge-parameter independent counterterms, we use the pinch technique [238–242]. In this prescription, we obtain gauge-parameter independent self-energies by adding an additional contribution Σ^{add} to Σ^{tad} such that the pinched self-energy Σ^{pinch} is given by²²

$$\begin{aligned} i\text{Re} \left(\Sigma_{h_i h_j}^{\text{pinch}}(p^2) \right) &= i\text{Re} \left(\Sigma_{h_i h_j}^{\text{tad}}(p^2) \right) + i\Sigma_{h_i h_j}^{\text{add}}(p^2) \\ &= i\text{Re} \left(\Sigma_{h_i h_j}^{\text{tad}}(p^2) \right) \Big|_{\xi=1} \\ &\quad + -\frac{g^2}{32\pi^2 \cos^2 \theta_W} k_i k_j \left(p^2 - \frac{m_{h_i}^2 + m_{h_j}^2}{2} \right) \\ &\quad \times \left(B_0(p^2, m_Z^2, m_Z^2) + 2 \cos^2 \theta_W B_0(p^2, m_W^2, m_W^2) \right). \end{aligned} \quad (15.28)$$

Here, ξ ($\xi \in [\xi_W, \xi_Z]$) denote the gauge parameters and the coupling modifiers k_i ($i \in [1, 2]$) are defined in Eq. (2.41) and B_0 is the Passarino-Veltman two-point function [232, 245, 246]. In the counterterm $\delta\alpha$ we have implemented two different choices for the mass scale, which are the OS scheme, i.e. $p^2 = m_{h_i}^2$ ($i \in [1, 2]$), and the p^* scheme, i.e.

$$p^2 = p^* \equiv \frac{m_{h_1}^2 + m_{h_2}^2}{2}. \quad (15.29)$$

Therefore, the counterterm $\delta\alpha$ for the different choices is given by

$$\begin{aligned} \delta\alpha_{p^*} &= \frac{1}{m_{h_1}^2 - m_{h_2}^2} \text{Re} \left(\Sigma_{h_1 h_2}^{\text{tad}}(p^*) \Big|_{\xi=1} \right), \\ \delta\alpha_{\text{OS}} &= \frac{1}{2(m_{h_1}^2 - m_{h_2}^2)} \text{Re} \left(\Sigma_{h_1 h_2}^{\text{pinch}}(m_{h_1}^2) + \Sigma_{h_2 h_1}^{\text{pinch}}(m_{h_2}^2) \right). \end{aligned} \quad (15.31)$$

Renormalization of the Singlet VEV v_s

As with the previous parameters, we split the bare singlet VEV $v_{s,0}$ into a renormalized parameter and a counterterm, so that it is given by

$$v_{s,0} = v_s + \delta v_s. \quad (15.32)$$

We use for the renormalization of v_s the process-dependent scheme [9, 243, 244]. In order to fix the counterterm δv_s , we use a physical process and demand that the renormalized singlet VEV is determined by the LO relation, while the higher-order corrections are taken into account by the counterterm. The process-dependent counterterm is obtained by using a decay, where we demand the following condition

$$\Gamma^{\text{LO}} = \Gamma^{\text{NLO}}. \quad (15.33)$$

Here, Γ^{LO} and Γ^{NLO} denote the decay width at leading and next-to-leading order, respectively. Furthermore, the tree-level process must be dependent on v_s . In the CxSM, only scalar decays

²²For a more detailed description of this technique, we refer to Ref. [9, 243, 244]

come into question. In our analysis, we used the scalar decay of a Higgs h_i ($i \in [1, 2]$) into a dark matter pair (AA). Equation (15.33) leads to

$$0 = \text{Re}((\mathcal{M}_{h_i \rightarrow AA}^{\text{LO}})^* \mathcal{M}_{h_i \rightarrow AA}^{\text{NLO}}), \quad (15.34)$$

where $\mathcal{M}_{h_i \rightarrow AA}^{\text{LO}}$ and $\mathcal{M}_{h_i \rightarrow AA}^{\text{NLO}}$ are the amplitudes of the process $h_i \rightarrow AA$ at leading-order and next-to-leading order, respectively. As the leading-order amplitude is just a constant factor, Eq. (15.34) further reduces to

$$\begin{aligned} 0 &= \text{Re}(\mathcal{M}_{h_i \rightarrow AA}^{\text{NLO}}) = \text{Re}(\mathcal{M}_{h_i \rightarrow AA}^{\text{VC}}) + \text{Re}(\mathcal{M}_{h_i \rightarrow AA}^{\text{CT}}) \\ &= \text{Re}(\mathcal{M}_{h_i \rightarrow AA}^{\text{VC}}) - \lambda_{h_i AA} \left(\frac{\delta \lambda_{h_i AA}}{\lambda_{h_i AA}} + \delta Z_A + \frac{\delta Z_{h_i h_i}}{2} + \frac{\lambda_{h_j AA}}{\lambda_{h_i AA}} \frac{\delta Z_{h_j h_i}}{2} \right). \end{aligned} \quad (15.35)$$

Here, $\text{Re}(\mathcal{M}_{h_i \rightarrow AA}^{\text{VC}})$ and $\text{Re}(\mathcal{M}_{h_i \rightarrow AA}^{\text{CT}})$ denote the amplitudes for the virtual corrections and the counterterm contribution of this process, respectively, and $i, j \in \{1, 2\}$ ($i \neq j$). The trilinear coupling $\lambda_{h_i AA}$ is given by

$$\lambda_{h_i AA} = \frac{m_{h_i}^2}{v_s} \begin{cases} \sin \alpha, & i = 1 \\ \cos \alpha, & i = 2 \end{cases}, \quad (15.36)$$

which leads to the following counterterm

$$\frac{\delta \lambda_{h_i AA}}{\lambda_{h_i AA}} = \frac{\delta m_{h_i}^2}{m_{h_i}^2} - \frac{\delta v_s}{v_s} + T_i(\alpha) \delta \alpha, \quad T_i(\alpha) \equiv \begin{cases} \cot \alpha, & i = 1 \\ -\tan \alpha, & i = 2 \end{cases}. \quad (15.37)$$

As we have two possible decay widths, we have two possibilities to define the counterterm δv_s . For these, the final expressions of the counterterm δv_s read

$$\begin{aligned} \delta v_s^{h_1 \rightarrow AA} &= v_s \left(-\text{Re} \left(\frac{\mathcal{M}_{h_1 \rightarrow AA}^{\text{VC}}}{\lambda_{h_1 AA}} \right) + \frac{\delta m_{h_1}^2}{m_{h_1}^2} + \cot \alpha \delta \alpha + \delta Z_A \right. \\ &\quad \left. + \frac{\delta Z_{h_1 h_1}}{2} + \frac{\lambda_{h_2 AA}}{\lambda_{h_1 AA}} \frac{\delta Z_{h_2 h_1}}{2} \right), \\ \delta v_s^{h_2 \rightarrow AA} &= v_s \left(-\text{Re} \left(\frac{\mathcal{M}_{h_2 \rightarrow AA}^{\text{VC}}}{\lambda_{h_2 AA}} \right) + \frac{\delta m_{h_2}^2}{m_{h_2}^2} + \cot \alpha \delta \alpha + \delta Z_A \right. \\ &\quad \left. + \frac{\delta Z_{h_2 h_2}}{2} + \frac{\lambda_{h_1 AA}}{\lambda_{h_2 AA}} \frac{\delta Z_{h_1 h_2}}{2} \right). \end{aligned} \quad (15.38)$$

for the two processes. While this counterterm is gauge-parameter independent and leads to UV-finite results, we have a kinematical restriction on the parameter space, where we can only use this counterterm when the following condition is fulfilled

$$m_{h_i} > 2m_A. \quad (15.39)$$

In order to avoid this constraint, we implement the zero-momentum (ZEM) scheme [234], where the external momenta of the process $h_i \rightarrow AA$ are set to zero and we demand the following condition

$$0 = \text{Re}(\mathcal{M}_{h_i \rightarrow AA}^{\text{NLO}}(\{p^2 = 0\})). \quad (15.40)$$

This approach has been used in Ref. [247] in the context of the next-to-2HDM. For a more detailed description of the implementation in the CxSM, we refer to Ref. [234]. Note, that the

external leg corrections $\mathcal{M}_{h_i \rightarrow AA}^{\text{Leg}}(\{p^2 = 0\})$ are not exactly cancelled by the leg counterterms. Also the counterterms are now gauge-dependent. To cure this issue, we use the pinched self-energies in the definition of the wave function renormalization constants δZ . Finally, the counterterms δv_s^{ZEM} in the ZEM scheme for the two possible decay read

$$\begin{aligned}\delta v_s^{\text{ZEM}, h_1 \rightarrow AA} &= v_s \left(-\text{Re} \left(\frac{\mathcal{M}_{h_1 \rightarrow AA}^{\text{VC}}(\{p^2 = 0\}) + \mathcal{M}_{h_1 \rightarrow AA}^{\text{Leg}}(\{p^2 = 0\})}{\lambda_{h_1 AA}} \right) \right. \\ &\quad \left. + \cot \alpha \delta \alpha - \delta Z_A - \frac{2 \delta m_A^2}{m_A^2} - \frac{\delta Z_{h_1 h_1}^{\text{pinched}}}{2} - \tan \alpha \frac{\delta Z_{h_1 h_2}^{\text{pinched}}}{2} \right), \\ \delta v_s^{\text{ZEM}, h_2 \rightarrow AA} &= v_s \left(-\text{Re} \left(\frac{\mathcal{M}_{h_2 \rightarrow AA}^{\text{VC}}(\{p^2 = 0\}) + \mathcal{M}_{h_2 \rightarrow AA}^{\text{Leg}}(\{p^2 = 0\})}{\lambda_{h_2 AA}} \right) \right. \\ &\quad \left. - \tan \alpha \delta \alpha - \delta Z_A - \frac{2 \delta m_A^2}{m_A^2} - \frac{\delta Z_{h_2 h_2}^{\text{pinched}}}{2} - \tan \alpha \frac{\delta Z_{h_2 h_1}^{\text{pinched}}}{2} \right).\end{aligned}$$

15.3. Electroweak and Fermionic Sector

For the one-loop calculation presented in this work, we also need to renormalize the electroweak and fermionic sector. We will start the description with the massive gauge bosons $W^\pm$ and Z .

Renormalization of the Masses and Wave Functions of the Massive Gauge Bosons

For the mass counterterms of the massive gauge bosons and the wave function renormalization constants, we can use the OS renormalization described in Sec. 15.1, so that they are given by [232, 233].

$$\begin{aligned}\delta m_V^2 &= \text{Re}(\Sigma_V^{T, \text{tad}}(m_V^2)), \quad V = W, Z \\ \delta Z_{VV} &= -\text{Re} \left(\frac{\partial \Sigma_{VV}^{T, \text{tad}}(p^2)}{\partial p^2} \Big|_{p^2=m_V^2} \right), \\ \delta Z_{\gamma\gamma} &= -\text{Re} \left(\frac{\partial \Sigma_{\gamma\gamma}^T(p^2)}{\partial p^2} \Big|_{p^2=0} \right), \\ \delta Z_{Z\gamma} &= \frac{2}{m_Z^2} \text{Re}(\Sigma_{Z\gamma}^T(0)), \\ \delta Z &= -\frac{2}{m_Z^2} \text{Re}(\Sigma_{\gamma Z}^T(m_Z^2)),\end{aligned}\tag{15.41}$$

Here, the superscript T denotes the transverse part of the vector boson self-energy.

Renormalization of the Masses and Wave Functions of the Massive Fermions

In order to apply the OS scheme in the fermionic sector, we first need to write the renormalized self-energy $\hat{\Sigma}_f$ of a fermion f in terms of the renormalized scalar $\text{Re}(\hat{\Sigma}_f^S(p^2))$, the right-handed $\text{Re}(\hat{\Sigma}_f^R(p^2))$ and left-handed $\text{Re}(\hat{\Sigma}_f^L(p^2))$ self-energies, so that it reads

$$\text{Re}(\hat{\Sigma}_f(p^2)) = \not{p} P_L \text{Re}(\hat{\Sigma}_f^L(p^2)) + \not{p} P_R \text{Re}(\hat{\Sigma}_f^R(p^2)) + m_f \text{Re}(\hat{\Sigma}_f^S(p^2)).\tag{15.42}$$

Here P_L and P_R are the projection operators, which are given by

$$P_{L,R} = \frac{1 \mp \gamma_5}{2}. \quad (15.43)$$

After applying the OS conditions to Eq. (15.42), we obtain the mass counterterm δm_f^2 , and the left- and right- handed wave function renormalization constants δZ_f^L and δZ_f^R , respectively. They are given by [232]

$$\begin{aligned} \delta m_f &= \frac{m_f}{2} \text{Re} \left(\Sigma_f^{\text{tad},L}(m_f^2) + \Sigma_f^{\text{tad},R}(m_f^2) + 2\Sigma_f^{\text{tad},S}(m_f^2) \right), \\ \delta Z_f^R &= -\text{Re} \left(\Sigma_f^{\text{tad},R}(m_f^2) \right) - m_f \text{Re} \left(\frac{\partial}{\partial p^2} \left(\Sigma_f^{\text{tad},L}(p^2) + \Sigma_f^{\text{tad},R}(p^2) + 2\Sigma_f^{\text{tad},S}(p^2) \right) \right) \Big|_{p^2=m_f^2}, \\ \delta Z_f^L &= -\text{Re} \left(\Sigma_f^{\text{tad},L}(m_f^2) \right) - m_f \text{Re} \left(\frac{\partial}{\partial p^2} \left(\Sigma_f^{\text{tad},L}(p^2) + \Sigma_f^{\text{tad},R}(p^2) + 2\Sigma_f^{\text{tad},S}(p^2) \right) \right) \Big|_{p^2=m_f^2}. \end{aligned} \quad (15.44)$$

Renormalization of the Electric Charge e

In order to renormalize the electroweak VEV, we have shown that the counterterm δv is dependent on the mass counterterms of the massive gauge bosons $V = W^\pm, Z$ and the counterterm of the electric charge δZ_e . The electric charge is defined by the $e^+e^-\gamma$ coupling for OS external particles in the Thomson limit, i.e., the fine structure constant $\alpha(Q)$ is evaluated at $Q = 0$. This implies that the vertex corrections vanish OS and for zero momentum transfer. We can write the counterterm of the electric charge in terms of the transverse photon-photon and photon- Z self-energies, which is therefore given by [232, 233]

$$\delta Z_e^{\alpha(0)} = \frac{1}{2} \frac{\partial \Sigma_{\gamma\gamma}^T(p^2)}{\partial p^2} \Big|_{p^2=0} + \frac{\sin \theta_W}{\cos \theta_W} \frac{\Sigma_{\gamma Z}^T(0)}{m_Z^2}. \quad (15.45)$$

Note that the sign of the second term in Eq. (15.45) differs from the corresponding expression given in Ref. [232]. This discrepancy originates from a different sign convention adopted for the covariant derivative. Evaluating the finestructure constant α in the Thomson limit, leads to large logarithmic values, which stem from light fermion contributions. To cure this problem, we employ the G_μ scheme [248]. In this scheme the electroweak constant α_{EW} is defined in terms of the Fermi constant G_μ such that

$$\alpha_{G_\mu} = \frac{\sqrt{2}G_\mu m_W^2}{\pi} \left(1 - \frac{m_W^2}{m_Z^2} \right). \quad (15.46)$$

Double counting is avoided by subtracting the corrections that are absorbed in the leading-order process from the explicit corrections of order α . This is achieved by subtracting the weak corrections, denoted by Δr , to the muon decay [249, 250] from the corresponding corrections in the $\alpha(0)$ scheme. The counterterm of the electric charge is then given by

$$\delta Z_e|_{G_\mu} = \delta Z_e|_{\alpha(0)} - \frac{1}{2}(\Delta r)_{1\text{-loop}}, \quad (15.47)$$

where the explicit one-loop expression $(\Delta r)_{1\text{-Loop}}$ for Δr reads

$$\begin{aligned} (\Delta r)_{1\text{-loop}} &= \frac{\partial \Sigma_{\gamma\gamma}^T(k^2)}{\partial k^2} \Big|_{k^2=0} - \frac{\cos \theta_W^2}{\sin \theta_W^2} \left(\frac{\Sigma_{ZZ}^T(m_Z^2)}{m_Z^2} - \frac{\Sigma_{WW}^T(m_W^2)}{m_W^2} \right) + \frac{\Sigma_{WW}^T(0) - \Sigma_{WW}^T(m_W^2)}{m_W^2} \\ &\quad - 2 \frac{\cos \theta_W}{\sin \theta_W} \frac{\Sigma_{\gamma Z}^T(0)}{m_Z^2} + \frac{\alpha}{4\pi \sin \theta_W^2} \left(6 + \frac{7 - 4 \sin \theta_W^2}{2 \sin \theta_W^2} \log \cos \theta_W^2 \right). \end{aligned}$$

15.4. Parameter Conversion between Renormalization Schemes

We can estimate the theoretical uncertainty arising from missing higher-order corrections by changing the renormalization scheme (cf. Ref. [251]). To do so, we have to convert the input parameters to the new scheme. In the following, we will denote the renormalized parameter and the corresponding counterterm in the i -th renormalization scheme as p_i and δp_i , respectively. Furthermore, the bare parameter p_0 is independent of the renormalization scheme, which means we can obtain a relation between the different renormalization schemes by

$$p_0 = p_1 + \delta p_1(p_1) \stackrel{!}{=} p_2 + \delta p_2(p_2) . \quad (15.48)$$

If we are now interested in the renormalized parameters in the second scheme, we can expand Eq. (15.48) up to one-loop order, and express it in terms of the known renormalized parameter p_1 , so that it reads

$$p_2 \approx p_1 + \delta p_1(p_1) - \delta p_2(p_1) + \mathcal{O}(\delta p^2) . \quad (15.49)$$

15.5. Infrared Divergences

As we consider in the calculation of the relic density final states with electric and color charge, photons, and gluons appear in the loop diagrams. These types of diagrams lead to infrared divergences. According to the Kinoshita-Lee-Nauenberg theorem, IR safety is guaranteed upon including real corrections [252, 253]. The total UV- and IR-convergent cross section is then given by

$$\sigma_{\text{total}} = \underbrace{\int |\mathcal{M}_{\text{LO}}|^2 d\Pi_2}_{\sigma_{\text{LO}}} + 2 \underbrace{\int \text{Re}(\mathcal{M}_{\text{LO}} \mathcal{M}_{\text{1Loop}}^*) d\Pi_2}_{\sigma_{\text{virt}}} + \underbrace{\int |\mathcal{M}_{\text{real}}|^2 d\Pi_3}_{\sigma_{\text{real}}} . \quad (15.50)$$

Here, σ_{LO} , σ_{virt} , and σ_{real} denote the leading-order, the virtual, and the real emission cross section. Note, that in the matrix element $\mathcal{M}_{\text{1Loop}}$ denotes the renormalized amplitude, i.e., the loop and counterterm contributions are included here. The Lorentz-invariant phase space measures are given by $d\Pi_2$ and $d\Pi_3$, where the index indicates how many particles are in the final state.

While the Eq. (15.50) is infrared finite, the virtual and real emission cross sections are separately infrared divergent. The IR divergences arise in virtual corrections involving massless gauge bosons, such as photons or gluons, in loop diagrams. In particular, they enter through the IR-divergent derivatives of the self-energies, which are used in the wave function renormalization constants (cf. Eqs. (15.6), (15.8)), as well as through triangle diagrams with a massless particle in the loop. In the case of the real corrections, the IR divergences stem from the divergent phase space of the emitted massless gauge boson in the soft limit, where the momentum of the emitted particle becomes very small. To obtain a Lorentz-invariant cancellation of the IR divergences, dimensional regularization should be applied, such that the integration over phase space must be performed in $D = 4 - 2\epsilon$ dimensions. However, since it is very difficult to analytically extract the IR poles from the $2 \rightarrow 3$ phase-space integral to cancel them with the corresponding IR poles from the virtual corrections, this method is not suitable for numerical applications. Hence, we will use the Catani-Seymour dipole subtraction method [254], which we will discuss in Sec. 15.5.2. In order to use this method, we need to calculate the real corrections in the full three-body phase space $d\Pi_3$. For this purpose, we will give a brief overview of the derivation of the three-body phase space.

15.5.1. Phase Spaces

The $2 \rightarrow n$ annihilation cross section is composed of the flux factor F , the transition matrix element $\mathcal{M}_{2 \rightarrow n}$, and the phase space integration $d\Pi_n$. The phase space is dependent on the number of the considered final states and reads for a process for n final state particles as [152]

$$d\Pi_n(P; q_1, \dots, q_n) = \delta^4 \left(P - \sum_{i=1}^n q_i \right) \prod_{i=1}^n \frac{d^3 k_i}{(2\pi)^3 2E_i}, \quad (15.51)$$

where P is the total momentum of the initial state particles, and k_i and E_i denote the four-momentum and energy of the i -th final state particle. In this work, we consider the $2 \rightarrow 2$ annihilation and, for real corrections, the $2 \rightarrow 3$ annihilation process, in which one of the final-state particles radiates a photon or gluon. To calculate these real corrections, we first need to establish a framework for computing the three-body phase space. Here, we will follow the description of [255].

Three-Body Phase Space

We consider the most general $2 \rightarrow 3$ process, denoted as

$$p_1(m_a) + p_2(m_b) \rightarrow q_1(m_1) + q_2(m_2) + q_3(m_3), \quad (15.52)$$

where p_i ($i \in [1, 2]$) and q_j ($j \in [1, 2, 3]$) denote the four momenta of the initial and final states, respectively. Furthermore, the masses of the initial state particles are denoted by m_a and m_b , while the masses of the final state particles are denoted by m_j ($j \in [1, 2, 3]$). The differential cross section for this process is then given by

$$d\sigma = \frac{F}{(2\pi)^5} |\mathcal{M}|^2 \delta^4(p_a + p_b - \sum_i q_i) \frac{d^3 q_1}{2E_1} \frac{d^3 q_2}{2E_2} \frac{d^3 q_3}{2E_3}, \quad (15.53)$$

where delta distribution δ^4 ensures the energy and momentum conservation given by

$$p_1 + p_2 = q_1 + q_2 + q_3, \quad (15.54)$$

the flux factor F is given by

$$F = \frac{1}{4\sqrt{(p_1 + p_2)^2 - m_a^2 m_b^2}}, \quad (15.55)$$

and the energies of the final-state particles are denoted by E_i ($i \in [1, 2, 3]$).

In Fig. 15.1, we show the kinematics in the center-of-mass frame of the initial state particles. The four-momenta of the incoming particles then read

$$p_a = \begin{pmatrix} \frac{m_a^2 - m_b^2 + s}{2\sqrt{s}} \\ 0 \\ 0 \\ \sqrt{\frac{(m_a^2 - m_b^2 + s)^2}{4s} - m_a^2} \end{pmatrix}, \quad p_b = \begin{pmatrix} \frac{-m_a^2 + m_b^2 + s}{2\sqrt{s}} \\ 0 \\ 0 \\ -\sqrt{\frac{(m_a^2 - m_b^2 + s)^2}{4s} - m_a^2} \end{pmatrix} \quad (15.56)$$

Here, s denotes the Mandelstam variable, which reads

$$s = (p_1 + p_2)^2 = (q_1 + q_2 + q_3)^2. \quad (15.57)$$

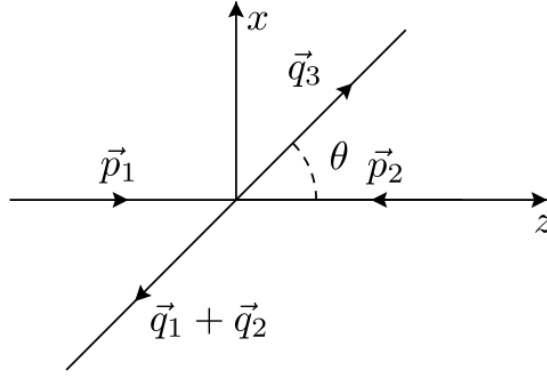


Figure 15.1.: Kinematics in the center-of-mass frame of the initial state particles. Taken from Ref. [255].

The energy E_3 of the third outgoing particle is given by

$$E_3 = \sqrt{|\vec{q}_3|^2 + m_3^2}, \quad (15.58)$$

which means we can perform a change of variables in Eq. (15.53), so that it reads

$$|\vec{q}_3|^2 d|\vec{q}_3| = 2dE_3 \sqrt{E_3^2 - m_3^2}. \quad (15.59)$$

The cross section can then be written in terms of the energy of the third outgoing particle and the scattering angle θ

$$\begin{aligned} \sigma = & \frac{F}{2^5 \pi^4} \int_0^\pi \sin \theta d\theta \int_{m_3^2}^{E_{3,\max}} \sqrt{E_3^2 - m_3^2} dE_3 \\ & \times \underbrace{\int \frac{d^3 q_1}{2E_1} \frac{d^3 q_2}{2E_2} \delta^4(p_1 + p_2 - q_1 - q_2 - q_3) |\mathcal{M}|^2}_{X}. \end{aligned} \quad (15.60)$$

Note that we integrated already over the azimuthal angle φ , which can trivially be done, as the scattering is located in a plane. To proceed, we first need to evaluate the Lorentz-invariant integral X . We can perform the integration in the center-of-mass frame of the first and second outgoing particles. The invariant mass m_{12}^2 of that pair is given by

$$m_{12}^2 = (q_1 + q_2)^2 = (p_1 + p_2 - q_3) = s + m_3^2 - 2\sqrt{s}E_3. \quad (15.61)$$

After integration over $d^3 q_2$, the integral X is then given in terms of the momenta q_i^* ($i \in [1, 2]$) in the center-mass frame of the outgoing particles by

$$\begin{aligned} X = & \frac{1}{4} \int \frac{d^3 q_1^*}{E_1^* E_2^*} \delta(m_{12} - E_1 - E_2) |\mathcal{M}|^2 \\ = & \frac{1}{4} \int \frac{|\vec{q}_1^*|^2 d|\vec{q}_1^*| d\Omega_1^*}{E_1^* E_2^*} \delta(m_{12} - E_1^* - E_2^*) |\mathcal{M}|^2. \end{aligned} \quad (15.62)$$

The energies E_1^* and E_2^* given by

$$E_1^* = \sqrt{|\vec{q}_1^*|^2 + m_1^2}, \quad E_2^* = \sqrt{|\vec{q}_1^*|^2 + m_2^2}, \quad (15.63)$$

where we used that $|\vec{q}_1^*| = |\vec{q}_2^*|$, and $d\Omega_1^*$ denotes the solid angle integration measure is given by $d\Omega_1^* = \sin \theta^* d\theta^* d\varphi^*$. The integral X can then be evaluated as

$$\begin{aligned}
X &= \frac{1}{4} \int \frac{|\vec{q}_1^*|^2 d|\vec{q}_1^*| d\Omega_1^*}{E_1^* E_2^*} \delta(m_{12} - \sqrt{|\vec{q}_1^*|^2 + m_1^2} - \sqrt{|\vec{q}_1^*|^2 + m_2^2}) |\mathcal{M}|^2 \\
&= \frac{1}{4} \int d\Omega_1^* \frac{|\vec{q}_1^*|^2}{E_1^* E_2^*} \frac{1}{|\vec{q}_1^*| \frac{E_1^* + E_2^*}{E_1^* E_2^*}} |\mathcal{M}|^2 \\
&= \frac{1}{4} \frac{|\vec{q}_1^*|}{m_{12}} \int d\Omega_1^* |\mathcal{M}|^2 \\
&= \frac{1}{8} \frac{\lambda(m_{12}, m_1, m_2)}{m_{12}^2} \int d\Omega_1^* |\mathcal{M}|^2.
\end{aligned} \tag{15.64}$$

Here, we used that the absolute value of the three-momentum $|\vec{q}_1^*|$ is given in terms of the Källén function λ as

$$|\vec{q}_1^*| = \frac{\lambda(m_{12}, m_1, m_2)}{2m_{12}^2}. \tag{15.65}$$

Inserting Eq. (15.64) into Eq. (15.60), we obtain the final form of the cross section which reads

$$\begin{aligned}
\sigma &= \frac{1}{64(2\pi)^4} \frac{1}{\sqrt{(p_1 \cdot p_2)^2 - m_a^2 m_b^2}} \int_{m_3}^{E_{3,\max}} dE_3 \sqrt{E_3 - m_3^2} \int_0^\pi d\theta \sin \theta \\
&\quad \times \int_0^\pi d\theta^* \sin \theta^* \int_0^{2\pi} d\varphi^* \frac{\lambda(m_{12}, m_1, m_2)}{2m_{12}^2} |\mathcal{M}|^2.
\end{aligned} \tag{15.66}$$

Note that the cross section is given in two different coordinates. However, as the center-of-mass system of the final state pair $\{q_1, q_2\}$ (CM*) is moving away from the center-of mass system of the initial state pair $\{p_1, p_2\}$ (CM) at an angle θ with a velocity β , we can relate the four-vectors in CM* to the four-vectors in CM by a Lorentz transformation. We can parametrize the four-vectors q_1^* and q_2^* as follows

$$q_1^* = \begin{pmatrix} E_1^* \\ |\vec{q}_1^*|_z \sin \theta^* \cos \varphi^* \\ |\vec{q}_1^*|_z \sin \theta^* \sin \varphi^* \\ |\vec{q}_1^*|_z \cos \theta^* \end{pmatrix}, \quad q_2^* = \begin{pmatrix} E_2^* \\ -|\vec{q}_1^*|_z \sin \theta^* \cos \varphi^* \\ -|\vec{q}_1^*|_z \sin \theta^* \sin \varphi^* \\ -|\vec{q}_1^*|_z \cos \theta^* \end{pmatrix}. \tag{15.67}$$

In order to evaluate the scalar products, which appear in the squared matrix element $|\mathcal{M}|^2$, all four-momenta need to be in the same reference frame. Therefore, we perform a Lorentz transformation on the four-momenta in Eq. (15.67) into CM, where the Lorentz transformation is given by

$$q_i = R_y(\theta + \pi) B_z(\gamma) q_i^*. \tag{15.68}$$

Here, $R_y(\theta + \pi)$ is a rotation matrix around the y -axis and $B_z(\gamma)$ corresponds to a boost in the z -direction as a function of the Lorentz factor γ . The matrices read

$$B_z = \begin{pmatrix} \gamma & 0 & 0 & \gamma\beta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \gamma\beta & 0 & 0 & \gamma \end{pmatrix}, \quad R_y = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta & 0 & \sin \theta \\ 0 & 0 & 1 & 0 \\ 0 & -\sin \theta & 0 & \cos \theta \end{pmatrix}. \tag{15.69}$$

Here, $\beta = (1 - \gamma^{-2})^{1/2}$. The Lorentz factor γ is given by

$$\gamma = \frac{\sqrt{s} - E_3}{m_{12}}. \quad (15.70)$$

As a last step, we have to define the integration boundaries in Eq. (15.66), in particular, the integration range of the energy of the third particle E_3 . The lower bound $E_{3,\min} = m_3$ is trivially obtained due to Eq. (15.58). The upper limit is given by the maximum value of $|q_3|$, which can be expressed in CM by the center-of-mass energy s , which reads

$$s = (p_1 + p_2)^2 = (E_1 + E_2 + E_3)^2 = \left(\sqrt{|\vec{q}_1 + \vec{q}_2|^2 + m_{12}^2} + \sqrt{|\vec{q}_3|^2 + m_3^2} \right)^2 \quad (15.71)$$

$$\left(\sqrt{|\vec{q}_3|^2 + m_{12}^2} + \sqrt{|q_3|^2 + m_3^2} \right)^2.$$

Here, we used the fact that k_3 equals the negative sum of q_1 and q_2 in the CM. Inverting Eq. (15.71) yields

$$|\vec{q}_3| = \frac{\lambda(\sqrt{s}, m_{12}, m_3)}{2\sqrt{s}}. \quad (15.72)$$

Therefore $|\vec{q}_3|$ becomes maximal in the case, where $m_{12} = m_1 + m_2$, and hence the upper integration bound $E_{3,\max}$ is given by

$$E_{3,\max} = \sqrt{\frac{\lambda(\sqrt{s}, m_1 + m_2, m_3)^2}{4s}} + m_3. \quad (15.73)$$

15.5.2. Catani-Seymour Subtraction Method

In the following, we give an overview of the Catani-Seymour Subtraction method, where we follow the description in Ref. [254].²³ The dipole formalism, first developed for massless emitter particles in Ref. [257] and later generalized in Ref. [254], cures IR divergences via a subtraction method. The idea is to subtract an auxiliary cross section $d\sigma_A$, which has the same pointwise singular behavior as $d\sigma_{\text{real}}$, from the real corrections and add it to the virtual corrections. The difference $\sigma_{\text{real}} - \sigma_A$ is integrable over the whole $(m + 1)$ particle phase space, where m denotes the number of final state particles in the LO order calculation. In particular, it is possible to integrate this in any dimension, and we can safely go to the limit $\epsilon \rightarrow 0$. Furthermore, as the integration over the singular subspace $\int_1 d\sigma_A$ contains analytically all IR ϵ poles, which cancel those of the virtual corrections, also the sum $d\sigma_{\text{virt}} + \int_1 d\sigma_A$ is integrable in $d = 4$ dimension over the m particle phase space.

The total cross section σ_{total} is then given by

$$\sigma_{\text{total}} = \int_m d\sigma_{\text{LO}} + \int_{m+1} [d\sigma_{\text{real}} - d\sigma_A] + \int_m \left[d\sigma_{\text{virt}} + \int_1 d\sigma_A \right]. \quad (15.74)$$

Here, the indices of the integrals denote the m , $(m + 1)$ and the one-dimensional phase-space integrals. To construct the auxiliary cross section $d\sigma_A$ within the dipole formalism, we first need to define the individual contributions called dipoles. Each dipole represents the soft

²³Note, that this method was originally developed for the QCD case. Nevertheless, its extension to the electroweak case is straightforward. To explain the Catani-Seymour subtraction method, however, it is sufficient to demonstrate the Catani-Seymour subtraction formalism only in the QCD context, and the corresponding electroweak derivation will therefore not be presented explicitly. For a detailed overview of the electroweak case, we refer to Refs. [233, 256].

and/or collinear radiation from a specific parton pair. The first parton is the emitter particle, while the second parton is the spectator. The IR singularities are defined by the kinematics of the former. The idea is as follows: We use the Born-level cross section to produce an m -parton configuration, then select all possible combinations of emitter-spectator pairs. The emitter decays into two partons, while the spectator, which carries the color and spin correlation of the real correction, is used to maintain momentum conservation. The auxiliary cross section $d\sigma_A$ reads

$$d\sigma_A = \sum_{\text{dipoles}} d\sigma_{\text{LO}} \otimes dV_{\text{dipole}} \quad , \quad (15.75)$$

where dV_{dipole} are the dipole factors, which describe the two-parton decays of the emitter particles. We can use Eq. (15.75), because the QCD amplitudes factorize on soft and collinear poles. The product structure of Eq. (15.75) allows us to use a mapping from the $(m+1)$ phase space to an m subspace, which reads

$$\int_{m+1} d\sigma_A = \sum_{\text{dipoles}} \int_m \sigma_{\text{LO}} \otimes \int_1 dV_{\text{dipole}} = d\sigma_{\text{LO}} \otimes \mathbf{I} \quad , \quad (15.76)$$

where the universal factor $\mathbf{I}$ is defined as

$$\mathbf{I} = \sum_{\text{dipoles}} \int_1 dV_{\text{dipole}} \quad . \quad (15.77)$$

Note that the single-particle phase space is process-independent. It describes the decay of the dipole and captures the kinematic dependence on the degrees of freedom that give rise to the IR singularities. Furthermore, it exactly cancels all ϵ poles in the virtual contributions σ_{virt} . Using this, we obtain an expression for the next-to-leading order cross section σ_{NLO} , which reads

$$\sigma_{\text{NLO}} = \int_{m+1} \left[d\sigma_{\text{real}} - \sum_{\text{dipoles}} d\sigma_{\text{LO}} \otimes dV_{\text{dipole}} \right] + \int_m [d\sigma_{\text{virt}} + d\sigma_{\text{LO}} \otimes \mathbf{I}] \quad . \quad (15.78)$$

In the following, we will provide the explicit expressions for the dipole factor dV_{dipole} and $\mathbf{I}$. We will start with the former. The dipole factorization formula from Ref. [257] can be used in order to construct the auxiliary function $d\sigma_A$, which reads

$$d\sigma_A = \sum_{\{i,j\}} \sum_{k \neq i,j} \mathcal{D}_{ij,k}(q_1, \dots, q_{m+1}) \quad . \quad (15.79)$$

Here, the four-momentum of the respective particle i ($i \in [1, \dots, m+1]$) is given by q_i , and we sum over the pairs $\{i, j\}$, where i denotes the parent particle, j the emitted particle, and k the spectator particle. The dipoles $\mathcal{D}_{ij,k}$ are given by

$$\mathcal{D}_{ij,k}(q_1, \dots, q_{m+1}) = \frac{-1}{(q_i + q_j)^2 - m_{ij}^2} {}_m \langle \dots, \tilde{i}j, \dots, \tilde{k}, \dots | \frac{\mathbf{T}_k \cdot \mathbf{T}_{ij}}{\mathbf{T}_{ij}} \mathbf{V}_{ij,k} | \dots, \tilde{i}j, \dots, \tilde{k}, \dots \rangle_m \quad , \quad (15.80)$$

where $\mathbf{T}_a$ denote the color operators. We will return to the operator $\mathbf{V}_{ij,k}$ at a later stage. First, we want to emphasize that the color and helicity dependent amplitude $\mathcal{M}_m$ is written in terms of the basis $\{|c_1, \dots, c_m\rangle \otimes |s_1, \dots, s_m\rangle\}$ such that it reads

$$\mathcal{M}_m = (\langle c_1, \dots, c_m | \otimes \langle s_1, \dots, s_m |) |1, \dots, m\rangle_m \quad . \quad (15.81)$$

Note that in Eq. (15.80), the matrix element depends on the momenta of the partons $\tilde{i}j$ and $\tilde{k}$. We can identify $\tilde{i}j$ as the emitter parton, with a mass m_{ij} , which later radiates an emitter

particle j and propagates afterward as a parton i , while $\tilde{k}$ is identified as a spectator parton. The auxiliary momenta of the partons $\tilde{i}j$ and $\tilde{k}$, q_{ij}^μ and q_k^μ can be related to the original momenta q_i^μ , q_j^μ and q_k^μ and the total momenta $Q^\mu = q_i^\mu + q_j^\mu + q_k^\mu$ and are given by

$$\tilde{q}_k^\mu = \frac{\lambda(Q^2, m_{ij}^2, m_k^2)^{1/2}}{\lambda(Q^2, (q_i + q_j), m_k^2)^{1/2}} \left(q_k^\mu - \frac{Q q_k}{Q^2} Q^\mu \right) + \frac{Q^2 + m_k^2 - m_{ij}^2}{2Q^2} Q^\mu, \quad \tilde{q}_k^2 = m_k^2, \quad (15.82)$$

$$\tilde{q}_{ij}^\mu = Q^\mu - \tilde{q}_k^\mu, \quad \tilde{q}_{ij}^2 = m_{ij}^2. \quad (15.83)$$

For our purposes, we are looking at the following splitting process $\tilde{i}j \rightarrow i + j$

$$Q \rightarrow g(q_i) + Q(q_j) : m_i = 0 \quad \text{and} \quad m_j = m_{ij} = m_k = m_Q, \quad (15.84)$$

where Q denotes a massive quark and g denotes the emitted gluon. The mass of the spectator particle k is denoted by m_Q , since we are considering $Q\bar{Q}$ final states. Finally, the operator $\mathbf{V}_{ij,k}$ is then given by²⁴

$$\mathbf{V}_{ij,k} \equiv \mathbf{V}_{gQ,k} = 8\pi\mu^{2\epsilon}\alpha_S C_F \left\{ \frac{2}{1 - \tilde{z}_j(1 - y_{ij,k})} - \frac{\tilde{v}_{ij,k}}{v_{ij,k}} \left[1 + \tilde{z}_j + \frac{m_Q^2}{q_i q_j} + \epsilon(1 - \tilde{z}) \right] \right\}, \quad (15.85)$$

where $y_{ij,k}$ and $\tilde{z}_i$ are given by

$$y_{ij,k} = \frac{q_i q_k}{q_i q_j + q_i q_k + q_j q_k}, \quad \tilde{z}_i = 1 - \tilde{z}_j = \frac{q_i q_k}{q_i q_k + q_j q_k}, \quad (15.86)$$

and $\tilde{v}_{ij,k}$ are the relative velocities between $\tilde{q}_{ij}$ and q_k and $v_{ij,k}$ are the relative velocities between $q_i + q_j$ and p_k , μ is the renormalization scale and $C_F = 4/3$. The relative velocities are given by

$$\tilde{v}_{ij,k} = \frac{\lambda(1, \mu_{ij}^2, \mu_k^2)}{1 - \mu_{ij}^2 - \mu_k^2}, \quad \text{with} \quad \mu_n = \frac{m_n}{\sqrt{Q^2}}, \quad (15.87)$$

and

$$v_{ij,k} = \frac{\sqrt{[2\mu_k + (1 - \mu_i^2 - \mu_j^2 - \mu_k^2)(1 - y_{ij,k})]^2 - 4\mu_k^2}}{(1 - \mu_i^2 - \mu_j^2 - \mu_k^2)(1 - y_{ij,k})}. \quad (15.88)$$

Next, we want to obtain an expression for the integrated dipole $\mathbf{I}$ in Eq. (15.89) by considering first the integral

$$\int_1 d\sigma_A = {}_m\langle 1, \dots, m | \mathbf{I}(\epsilon, \mu^2; \{q_i, m_i\}) | 1, \dots, m \rangle_m. \quad (15.89)$$

Here, the operator $\mathbf{I}$ depends on the mass, the momenta, and the masses of the m final state partons, so that it reads

$$\begin{aligned} \mathbf{I} = & -\frac{\alpha_S}{2\pi} \frac{(4\pi)^\epsilon}{\Gamma(1-\epsilon)} \sum_{j=1}^m \frac{1}{\mathbf{T}_k^2} \sum_{k \neq j} \mathbf{T}_j \cdot \mathbf{T}_k \\ & \times \left[\mathbf{T}_j^2 \left(\frac{\mu^2}{2q_j q_k} \right)^\epsilon \left(\mathcal{V}_j(2q_j q_k, m_j, m_k, \epsilon) - \frac{\pi^2}{3} \right) + \Gamma_j(\mu, m_j, \epsilon) \right. \\ & \left. + \gamma_j \ln \frac{\mu^2}{2q_j q_k} + \gamma_j + K_j + \mathcal{O}(\epsilon) \right]. \end{aligned} \quad (15.90)$$

²⁴The expression here is actually the spin-averaged function, as in general $\mathbf{V}_{ij,k}$ is non-diagonal in helicity-space.

As we are only considering quarks in the final state, i.e., j is a quark, the constants γ_j and K_j are given by

$$\gamma_j = \frac{3}{2}C_F, \quad K_j = \left(\frac{7}{2} - \frac{\pi^2}{6}\right)C_F, \quad (15.91)$$

where $C_F = 4/3$. The kernel functions $\mathcal{V}$ can be decomposed into a singular part and a non-singular part, so that it reads

$$\mathcal{V}_j = V^S(s_{jk}, m_j, m_k, \epsilon) + \mathcal{V}^{\text{NS}}(s_{jk}, m_j, m_k), \quad (15.92)$$

where we introduced the short-hand notation $s_{jk} = 2q_j q_k$. Note, that we are considering that both particles j and k are massive quarks. The singular term is then given by

$$\begin{aligned} \mathcal{V}^S(s_{jk}, m_j, m_k, \epsilon) = & \frac{1}{v_{jk}} \left[\frac{1}{\epsilon} \ln \rho - \frac{1}{2} \ln^2 \rho_j - \frac{1}{2} \ln^2 \rho_k - \frac{\pi^6}{6} \right] \\ & + \frac{1}{v_{jk}} \ln \rho \ln \frac{s_{jk} + m_j^2 + m_k^2}{s_{jk}}, \end{aligned} \quad (15.93)$$

and the non-singular term is given by

$$\begin{aligned} \mathcal{V}^{\text{NS}}(s_{jk}, m_j, m_k) = & \frac{\gamma_j}{T_j^2} \ln \frac{s_{jk}}{Q_{jk}^2} \\ & + \frac{1}{v_{jk}} \left[2 \ln \rho \ln(1 + \rho^2) + 2 \text{Li}_2(\rho^2) - \text{Li}_2(1 - \rho_j^2) - \text{Li}_2(1 - \rho_k^2) - \frac{\pi^2}{6} \right] \\ & + \ln \frac{Q_{jk} - m_k}{Q_{jk}} - 2 \ln \frac{(Q_{jk} - m_k)^2 - m_j^2}{Q_{jk}^2} - \frac{2m_j^2}{s_{jk}} \ln \frac{m_j}{Q_{jk} - m_k} \\ & - \frac{m_k}{Q_{jk} - m_k} + \frac{2m_k(2m_k - Q_{jk})}{s_{jk}} + \frac{\pi^2}{2}, \end{aligned} \quad (15.94)$$

where we used the shorthand notation $Q_{jk}^2 \equiv s_{jk} + m_j^2 + m_k^2$ and ρ and ρ_n ($n \in [j, k]$) are given by

$$\rho_n = \sqrt{\frac{1 - v_{j,k} + 2\mu_n^2/(1 - \mu_j^2 - \mu_k^2)}{1 + v_{j,k} + 2\mu_n^2/(1 - \mu_j^2 - \mu_k^2)}} \quad \text{with } \mu_n^2 = \frac{m_n^2}{Q_{jk}^2}, \quad (15.95)$$

and

$$\rho = \sqrt{\frac{1 - v_{j,k}}{1 + v_{j,k}}}. \quad (15.96)$$

The function Γ_j is given by

$$\Gamma_j(\mu, m_Q, \epsilon) = C_F \left[\frac{1}{\epsilon} + \frac{1}{2} \ln \frac{m_Q^2}{\mu^2} - 2 \right], \quad (15.97)$$

where m_Q is the mass of quark j . Finally, by using

$$\sigma_{\text{NLO}} = \int_{m+1} [\text{d}\sigma_{\text{real}} - \text{d}\sigma_A] + \int_m [\text{d}\sigma_{\text{virt}} + \int_1 \text{d}\sigma_A] . \quad (15.98)$$

and inserting Eqs (15.79) and (15.89), we obtain UV- and IR-finite next-to-leading order cross sections.

In our analysis, we used **FeynCalc** [150] and **FeynArts** [147, 148] to generate the next-to-leading order annihilation amplitudes squared. The Passarino-Veltman functions are evaluated in **RelExt** via a link to the code **Collier** [258]. To discuss the influence of higher-order corrections on the relic abundance, we generated a sample of parameter points that satisfy all relevant theoretical and experimental constraints. These parameter points have been obtained by the public code **ScannerS** [18, 116]. In the following, we will briefly introduce the relevant theoretical and experimental constraints considered in this work and also provide the scan ranges of our parameter scan.

16.1. Theoretical Constraints

Boundedness from Below

We can obtain the conditions to have a stable minimum by writing the quartic terms of the potential given in Eq. (2.33) in terms of $x \equiv \Phi^\dagger \Phi$ and $y \equiv |\mathbb{S}|^2$,

$$V_{\text{quartic}}(x, y) = \frac{1}{4} \begin{pmatrix} x & y \end{pmatrix}^T \underbrace{\begin{pmatrix} \lambda & \delta_2 \\ \delta_2 & d_2 \end{pmatrix}}_{\equiv A} \begin{pmatrix} x \\ y \end{pmatrix}. \quad (16.1)$$

In order for the potential to be bounded from below, the matrix A needs to be copositive, which means that the conditions for the parameters are given by

$$\lambda > 0 \wedge d_2 > 0 \wedge (\delta_2^2 < \lambda d_2 \text{ if } \delta_2 < 0). \quad (16.2)$$

Perturbative Unitarity

We ensure perturbative unitarity by demanding that the eigenvalues λ_i of the scalar $2 \rightarrow 2$ scattering matrix fulfill the following condition [259]

$$|\lambda_i|^2 \leq 8\pi. \quad (16.3)$$

In the CxSM, this leads to the following conditions on the potential parameters [116],

$$\begin{aligned} |\lambda| &\leq 16\pi \wedge |d_2| \leq 16\pi \wedge |\delta_2| \leq 16\pi \\ \left| \frac{3\lambda}{2} + d_2 \pm \sqrt{\left(\frac{3}{2}\lambda - d_2\right)^2 + 2\delta_2^2} \right| &\leq 16\pi. \end{aligned} \quad (16.4)$$

Vacuum Stability

We demand that the global minimum of the potential is given by the electroweak minimum at $v = 246$ GeV. In general, the vacuum structure of the CxSM given by

$$\langle \Phi \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}, \quad \langle S \rangle = \frac{1}{\sqrt{2}}(v_s + iv_A). \quad (16.5)$$

In this work, we consider the vacuum configuration with $v_A = 0$ and $v, v_s \neq 0$. In Ref. [234], it has been shown that this minimum is the global minimum at tree level if

$$\delta_2^2 < \lambda d_2. \quad (16.6)$$

16.2. Experimental Constraints

Electroweak Precision Parameters

Due to the additional scalar particle in the CxSM, additional contributions appear in the self-energies of the gauge bosons. These lead to deviations from the SM predictions. These deviations can be parametrized by the oblique parameters S, T , and U [97]. We check via **ScannerS**, which uses a fit result, the compatibility of the theoretical and experimental values.

Higgs Searches

The measurements at the LHC of the discovered Higgs boson as well as the searches for additional scalar particles constrain the parameter space of the CxSM. In order to obtain valid parameter points, **ScannerS** is linked to the public code **HiggsTools** [109], which is a unification of the modules **HiggsSignals** [112] and **HiggsBounds** [260]. Here, we check the agreement of the signal rates of the SM-like Higgs boson with the experimental data at the 2σ level by **HiggsSignals**. The constraints from the searches for the additional scalar particles in theory are included by **HiggsBounds**.

Dark Matter Observables

We impose that the parameter points must fulfill at leading-order the relic density constraint by the PLANCK experiment given in Eq. (3.22). This is checked with our code **RelExt** [129]. In the CxSM, the direct detection constraint does not affect the parameter space, as the LO cross section is suppressed by the small DM velocity and therefore negligible.

16.3. Parameter Scan

In this section, we provide the parameter ranges of our scan. The input parameters used are given in Eq. (2.45). We set the mass of one of the two visible particles to the experimentally measured value of the SM Higgs boson h , which reads [261]

$$m_h = 125.09 \text{ GeV}. \quad (16.7)$$

We scan the mass of the non-SM-like Higgs boson m_s in the range

$$126 \text{ GeV} \leq m_s \leq 1 \text{ TeV}. \quad (16.8)$$

The scan ranges of the DM mass m_A and the singlet VEV v_s are given by

$$62 \text{ GeV} \leq m_A \leq 1 \text{ TeV} , \quad (16.9)$$

and

$$1 \text{ GeV} \leq v_s \leq 1 \text{ TeV} . \quad (16.10)$$

We run the scan for the value of the mixing angle α in the range

$$-\frac{\pi}{2} \leq \alpha \leq \frac{\pi}{2} . \quad (16.11)$$

In the following chapter, we will present our results of the impact of the higher-order corrections on the relic abundance by performing a full electroweak and QCD next-to-leading order calculation of the annihilation amplitudes. To do so, we implemented the next-to-leading order squared annihilation amplitudes in the public code `RelExt`. Before we present our results, we want to give some general remarks on the relative corrections to the relic density.

17.1. Relative Correction to the Dark Matter Relic Abundance

The corrected relic density is given by

$$\Omega_{\text{corr}} = \Omega_{\text{LO}} + \Omega_{\text{NLO}} = \Omega_{\text{LO}} \left(1 + \frac{\Omega_{\text{NLO}}}{\Omega_{\text{LO}}} \right) = \Omega_{\text{LO}}(1 + \kappa_{\Omega}) , \quad (17.1)$$

where Ω_{LO} is the leading-order relic density and Ω_{NLO} is the pure next-to-leading order correction to the relic density, i.e., the sum of all virtual corrections, the counterterms, and the real corrections, where necessary. In Eq. (17.1), we introduced the relative correction to the relic density as

$$\kappa_{\Omega} \equiv \frac{\Omega_{\text{NLO}}}{\Omega_{\text{LO}}} . \quad (17.2)$$

The relic density is approximately inversely proportional to the thermally averaged cross section $\langle\sigma v\rangle$, so it reads

$$\Omega \sim \frac{1}{\langle\sigma v\rangle} . \quad (17.3)$$

The thermally averaged cross sections at leading-order and next-to-leading order are obtained by inserting the leading-order annihilation cross section σ_{ij}^{LO} and the next-to-leading-order annihilation cross section σ_{ij}^{NLO} into Eq. (9.30), respectively. Using this, we can obtain the following relation between the relative correction to the relic density and the corrections to the thermally averaged cross section

$$\kappa_{\Omega} = \frac{\Omega_{\text{corr}} - \Omega_{\text{LO}}}{\Omega_{\text{LO}}} \sim \frac{\frac{1}{\langle\sigma v\rangle^{\text{LO}} + \langle\sigma v\rangle^{\text{NLO}}} - \frac{1}{\langle\sigma v\rangle^{\text{LO}}}}{\frac{1}{\langle\sigma v\rangle^{\text{LO}}}} = \frac{1}{1 + \frac{\langle\sigma v\rangle^{\text{NLO}}}{\langle\sigma v\rangle^{\text{LO}}}} - 1 \equiv \frac{1}{1 + \kappa_{\sigma}} - 1 . \quad (17.4)$$

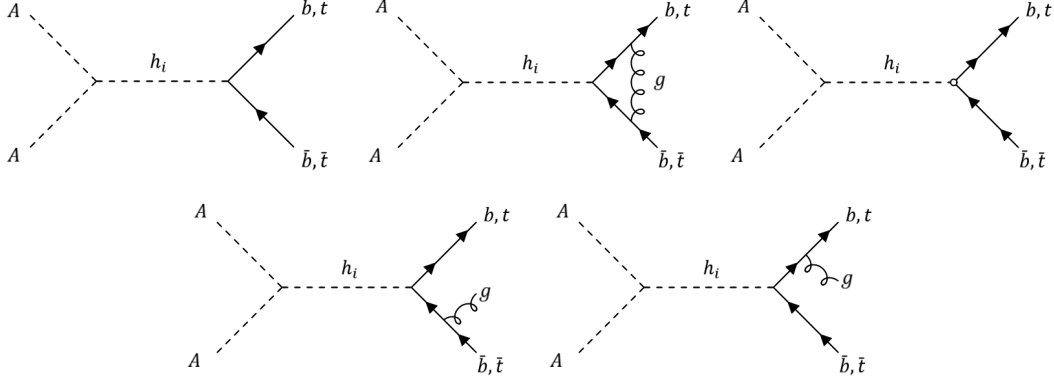


Figure 17.1.: Generic diagrams contributing of the dark matter annihilation process $AA \rightarrow q\bar{q}$ ($q = b, t$) at next-to-leading order QCD with the scalar Higgs mediators h_i ($i \in [1, 2]$). Top row: leading-order contribution (left), virtual vertex corrections (middle) and counterterm contribution (right). The white dot marks the counterterm insertion. Bottom row: Contributions of the real emission of a gluon g .

Here, we defined the relative corrections to the thermally averaged cross section as

$$\kappa_\sigma \equiv \frac{\langle \sigma v \rangle^{\text{NLO}}}{\langle \sigma v \rangle^{\text{LO}}} . \quad (17.5)$$

Equation (17.4) shows an important effect in our analysis. If we obtain negative relative corrections to the thermally averaged cross section, the relative corrections to the relic density grow very quickly. The relation is given by

$$\kappa_\sigma \in \{0, \dots, -1\} \quad \rightsquigarrow \quad \kappa_\Omega \in \{0, \dots, +\infty\} . \quad (17.6)$$

On the other hand, positive corrections to the thermally averaged cross section translate into a much lesser decrease in the corrections in the relic density, which cannot fall below -100% , which means

$$\kappa_\sigma \in \{0, \dots, +\infty\} \quad \rightsquigarrow \quad \kappa_\Omega \in \{0, \dots, -1\} . \quad (17.7)$$

17.2. Impact of the QCD Corrections on the Relic abundance

We begin by considering the impact of QCD corrections alone as a proof of concept, before turning to the complete next-to-leading order calculation including both electroweak and QCD contributions. In order to investigate the impact of the QCD corrections on the relic abundance, we implemented the QCD next-to-leading order annihilation amplitudes at order $\mathcal{O}(\alpha_s)$ in **RelExt**, which we introduced in Ch. 10. Note that only the third-generation quarks obtain QCD corrections at next-to-leading order, therefore, all other final states are calculated at leading-order, while the final states $t\bar{t}$ and $b\bar{b}$ are computed at next-to-leading order QCD. In Fig. 17.1, we show the generic diagrams contributing to the next-to-leading order QCD correction to the annihilation process $AA \rightarrow q\bar{q}$ ($q = b, t$).

In Fig. 17.2, we show κ_Ω as a function of the dark matter mass m_A . The color code for the parameter points indicates the channels, that dominantly contribute to the annihilation cross section, for each point. On the left plot, we show the mass range $62 \text{ GeV} \leq m_A \leq 120 \text{ GeV}$, while on the right plot, we present the mass range $120 \text{ GeV} \leq m_A \leq 1 \text{ TeV}$. At the mass range $60 \text{ GeV} \leq m_A \leq \sim 80 \text{ GeV}$, the dominant channel is the $b\bar{b}$ final state. Here, we see a correction of around 60%. We can understand these large corrections as follows: As the

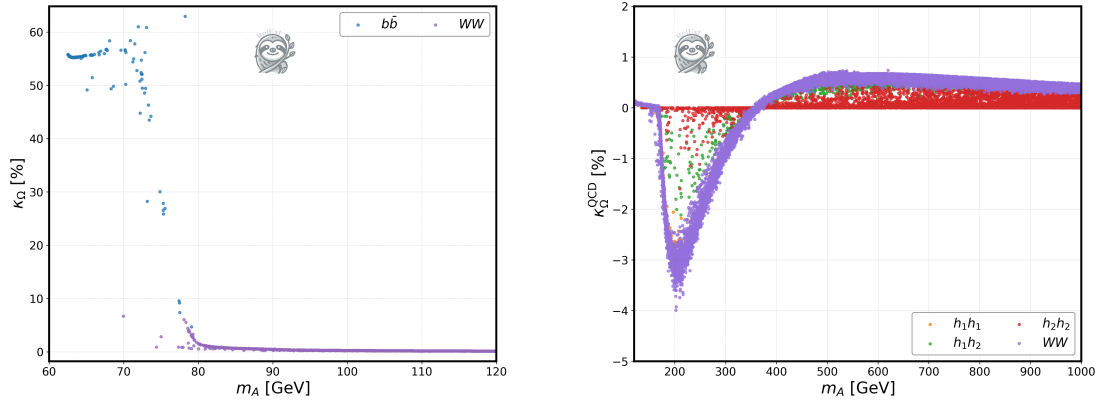


Figure 17.2.: Relative QCD corrections to the relic density, κ_Ω , as a function of the dark matter mass m_A for the mass ranges $62 \text{ GeV} \leq m_A \leq 120 \text{ GeV}$ (left) and $120 \text{ GeV} \leq m_A \leq 1 \text{ TeV}$ (right). The color code indicates the dominant channel in the annihilation cross section for the individual parameter point.

$b\bar{b}$ final state is the dominant channel in this regime, the thermally averaged cross section in Eq. (9.30) is dominated by the following term (ignoring the prefactors),

$$\langle\sigma v\rangle \propto \int_{4m_A^2}^{\infty} \sqrt{s} p_{ij}^2 \sigma_{b\bar{b}} K_1\left(\frac{\sqrt{s}}{m_A}x\right) ds, \quad (17.8)$$

where $\sigma_{b\bar{b}}$ denotes the annihilation cross section of the process $AA \rightarrow b\bar{b}$ at next-to-leading order. From the diagrams shown in Fig. 17.1, it can be seen that the QCD corrections are confined at the $h_i b\bar{b}$ ($i \in [1, 2]$) vertex, since neither the dark matter particle nor the Higgs mediators carry a color charge. Therefore, the QCD corrections κ_{QCD} can be factorized such that the cross section $\sigma_{b\bar{b}}$ is given by

$$\sigma_{b\bar{b}} = \sigma_{b\bar{b}}^{\text{LO}} (1 + \kappa_{\text{QCD}}), \quad (17.9)$$

where $\sigma_{b\bar{b}}^{\text{LO}}$ denotes the leading-order dark matter annihilation cross section into a $b\bar{b}$ pair. Note that the contribution of the non-SM like Higgs boson can be neglected, as its Yukawa coupling to a $b\bar{b}$ pair is suppressed by the mixing angle α . Furthermore, we consider scenarios in which the SM-like Higgs boson is the lighter of the two Higgs bosons, resulting in a further suppression of the s -channel contribution from the heavier, non-SM-like Higgs boson. The QCD corrections κ_{QCD} are therefore approximately equal to the QCD corrections $\kappa_{\text{QCD}}^{h_{\text{SM}} \rightarrow b\bar{b}}$ to the decay of the SM-like Higgs boson h_{SM} into a $b\bar{b}$ pair, which are known (c.f. Ref. [155]) and read

$$\kappa_{\text{QCD}}^{h_{\text{SM}} \rightarrow b\bar{b}} = C_F \frac{\alpha_s}{\pi} \left(\frac{9}{4} - \frac{3}{2} \log \left(\frac{m_h^2}{m_b^2} \right) \right) \approx -38\%. \quad (17.10)$$

Here, the color factor is given by $C_F = 4/3$, and the bottom quark mass is given by $m_b = 4.7 \text{ GeV}$ [152].²⁵ Inserting Eq. (17.10) into Eq. (17.4), we obtain approximately a correction of

$$\kappa_{\Omega, \text{QCD}} \approx 61.71\%, \quad (17.11)$$

which is in agreement with our results. Furthermore, at around $\sim 200 \text{ GeV}$, the next-to-leading order QCD corrections to the subdominant $t\bar{t}$ final state induce a $\sim -4\%$ correction

²⁵Note in the actual calculation we use the running $\overline{\text{MS}}$ bottom quark mass as described in Ch. 10. For this estimate, it suffices to use the bottom pole mass.

to the relic density. Note that in this parameter region the dominant annihilation channels are into W^+W^- or $h_i h_j$ ($i, j \in [1, 2]$) final states. Therefore, the QCD corrections do not have a significant impact on the relic density.

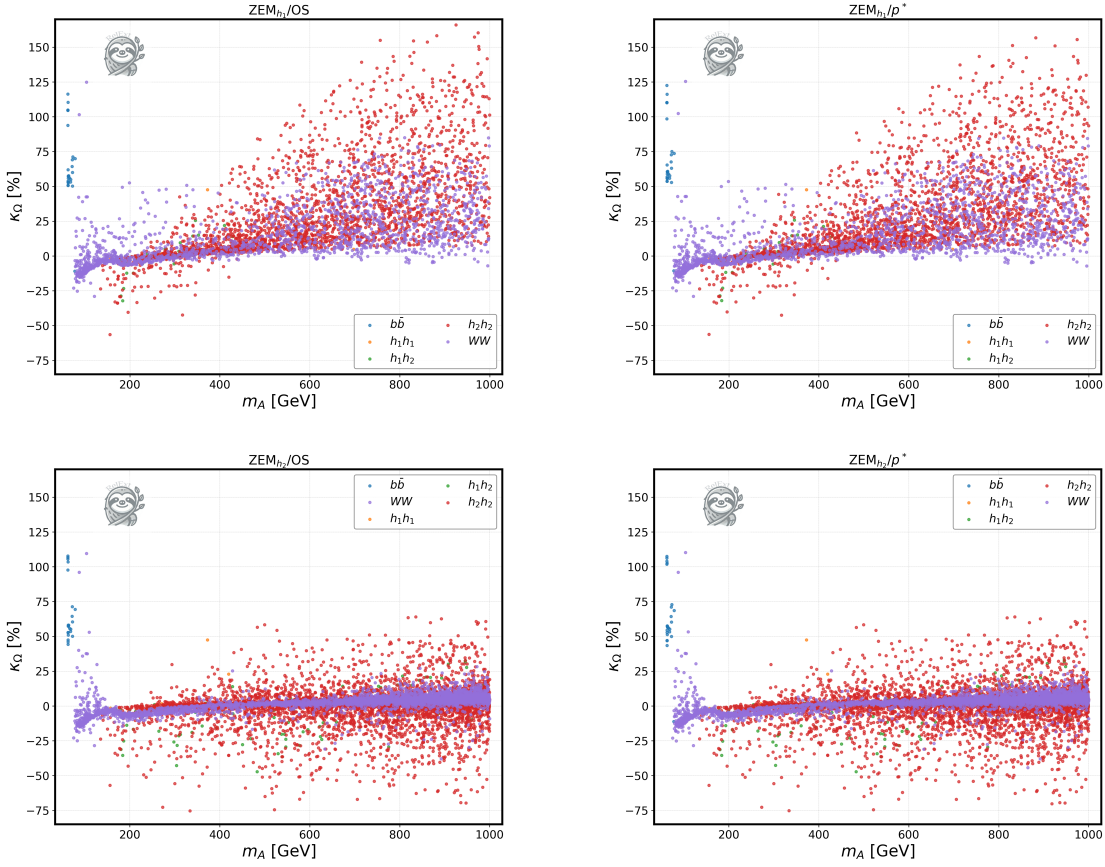


Figure 17.3.: Relative correction κ_Ω as a function of the dark matter mass m_A . The coloration of the points indicates the dominant annihilation channel. The color code is the following: W^+W^- (purple), h_2h_2 (red), h_1h_2 (orange), h_1h_1 (green), $b\bar{b}$ (blue). Upper: The chosen renormalization scheme on the left (right) for δv_s is the ZEM_{h_1} scheme and for α the OS-scheme (p^* scheme). Lower: The chosen renormalization scheme on the left (right) for δv_s is the ZEM_{h_2} scheme and for $\delta\alpha$ the OS-scheme (p^* scheme).

17.3. Impact of Electroweak and QCD Corrections on the Relic Abundance

In this section, we present the full next-to-leading order electroweak and QCD corrections on the dark matter relic abundance. In Fig. 17.3, we present the relative corrections κ_Ω as a function of the dark matter mass m_A . The coloration of each parameter point indicates the dominant annihilation channel. The dominant channels are annihilation into a W^+W^- pair (purple), a h_2h_2 (red) pair, a h_1h_2 (orange) final state, a h_1h_1 pair (green) and a $b\bar{b}$ pair (blue). Furthermore, in the upper row, we show the relative corrections, when using the ZEM_{h_1} scheme for the singlet VEV v_s and the OS-renormalization scheme (left) and the p^* -renormalization scheme (right) for the mixing angle α , while in the lower row, we instead used the ZEM_{h_2} scheme for δv_s . We observe that the change of renormalization schemes for α does not change the obtained results much. However, the choice of the renormalization of

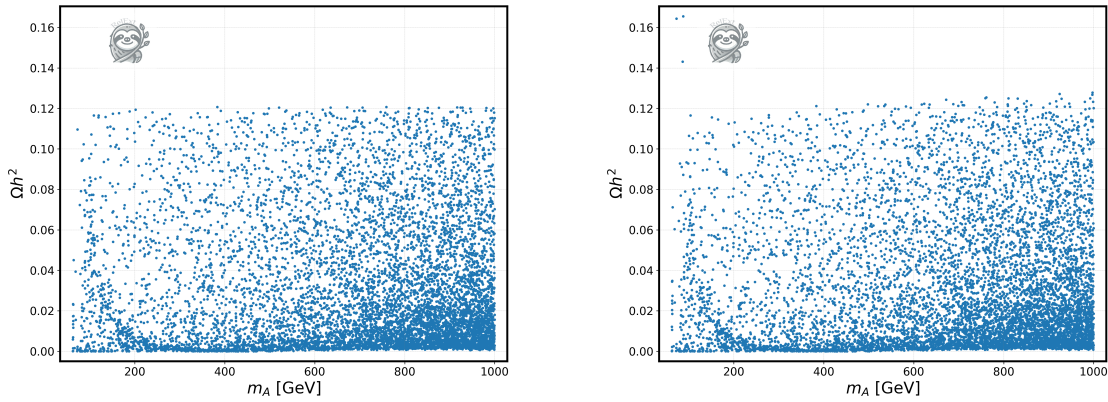


Figure 17.4.: The relic density Ωh^2 at leading-(left) and next-to-leading-order (right) as a function of the dark matter mass m_A .

the singlet VEV v_s can lead to very different results. Especially in the mass range $170 \text{ GeV} < m_A < 1000 \text{ GeV}$, the ZEM_{h_1} scheme can induce corrections to the relic density between -52% up to $\sim +160\%$. On the other hand, the ZEM_{h_2} scheme in the used parameter sample induces corrections between -75% and $+55\%$ in the same mass range. This behaviour is expected, as it was seen in Ref. [182] that using the ZEM_{h_1} scheme can lead to large next-to-leading-order corrections if the mass difference between h_1 and the dark matter particle $m_A - m_{h_1}$ becomes sizeable. In the range of $62.5 \text{ GeV} \leq m_A \leq 170 \text{ GeV}$ we obtain corrections up to $\sim +125\%$, using the ZEM_{h_1} scheme, while in the ZEM_{h_2} corrections go up to 110% . For masses near $m_A \approx m_h/2$, the dominant channel is the $b\bar{b}$ final state, where the corrections are driven by the QCD effects and are now also furthermore enhanced by the electroweak corrections. Overall, we can make the important observation here that the NLO corrections can both increase or decrease the computed relic density. In Fig. 17.4, we plot the relic density Ωh^2 over the dark matter mass m_A at leading-(left) and at next-to-leading-order (right). Note, that for the next-to-leading order calculation, we used for the renormalization of the singlet VEV v_s the ZEM_{h_2} scheme and α is renormalized in the OS-scheme. It can be observed that parameter points, which were previously valid, are invalid at next-to-leading order, since the relic density becomes larger than the measured value. This underlines the importance of the inclusion of higher-order corrections in the relic density calculation.

Uncertainty Estimate

Next, we want to investigate the theoretical uncertainty between two renormalization schemes. For this purpose, we introduce the parameter δ_{ren} [182], which reads

$$\delta_{\text{ren}}^\lambda = \frac{\Omega_{\text{corr}}^\lambda h^2 - \Omega_{\text{corr}}^{\text{ZEM}_{h_2}} h^2}{\Omega_{\text{corr}}^{\text{ZEM}_{h_2}} h^2}, \quad (17.12)$$

where $\Omega_{\text{corr}}^\lambda h^2$ is the relic density calculated at next-to-leading order in the renormalization scheme λ and $\Omega_{\text{corr}}^{\text{ZEM}_{h_2}} h^2$ is the relic density at next-to-leading order with v_s renormalized in the ZEM_{h_2} scheme and α in the OS scheme, which we will always assume as our reference input scheme. The input parameters need to be converted from the initial renormalization scheme to the new scheme via Eq. (15.48). In Tab. 17.1, we present the input parameters of the benchmark point BP1. Note, that the mixing angle α is renormalized in the OS scheme. We also show the converted input parameter $v_s^{\text{ZEM}_{h_1}}$ and the relic densities Ω_{LO} and Ω_{corr} as well as the relative correction κ_Ω in the ZEM_{h_1} and ZEM_{h_2} schemes. In this case, the theoretical uncertainty is $\delta_{\text{ren}}^{\text{ZEM}_{h_1}} = 1.18\%$. The reason is that the input parameter

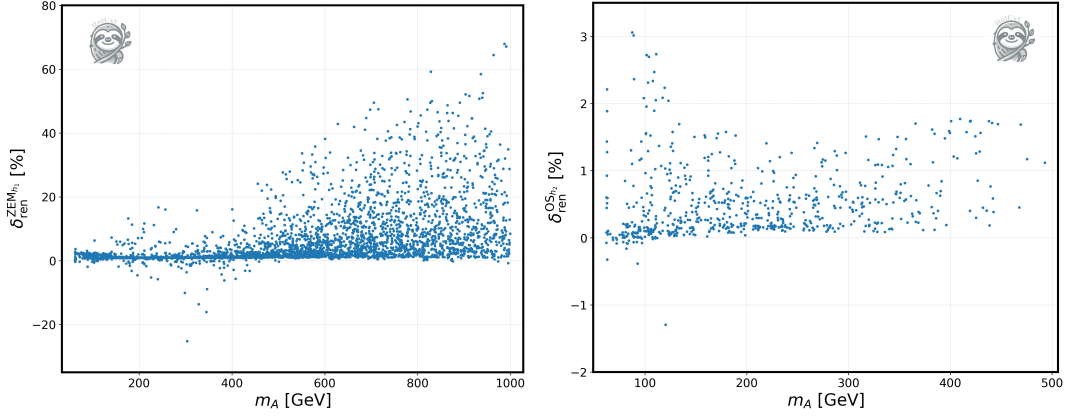


Figure 17.5.: Estimated uncertainty of the higher-order corrections to the relic density, $\delta_{\text{ren}}^{\text{ZEM}_{h1}}$ (left) and $\delta_{\text{ren}}^{\text{OS}_{h2}}$ (right), obtained from changing the renormalization scheme of v_S from the default ZEM_{h2} scheme to ZEM_{h1} and OS_{h2} , respectively, as a function of the DM mass. The right panel includes only parameter points with $m_{h2} > 2m_A$. Taken from Ref. [262].

v_s differs only slightly between the two schemes. Note that the leading-order relic density changes by $\sim -7\%$, due to the change of the singlet VEV v_s , however including the next-to-leading order corrections, the relic density values approach get closer to each other as expected. Since the leading-order relic density is smaller in the ZEM_{h1} scheme, the relative correction κ_Ω becomes larger. More specifically, the relative correction amounts to $\kappa_\Omega \approx 5.6\%$ in the ZEM_{h2} scheme, whereas it increases to $\kappa_\Omega \approx 14\%$ in the ZEM_{h1} scheme. Therefore, the ZEM_{h2} scheme constitutes the more suitable choice, as it exhibits a better perturbative convergence. In Tab. 17.2, we now change the renormalization scheme of the mixing angle to the p^* scheme for BP1. Note that now also the value of singlet VEV v_s changes as well, as it is dependent on the counterterm $\delta\alpha$ and therefore on its renormalization scheme. As the change in the renormalization scheme affects the input parameters only marginally, the theoretical uncertainty is small and amounts to $\delta_{\text{ren}}^{p^*} = 0.016\%$. As the leading-order relic density only changes slightly the relative correction in both schemes remain the same at $\kappa_\Omega \approx 5.6\%$.

Finally, we performed an uncertainty estimate for all parameter points included in our scan. Figure 17.5 shows the corresponding uncertainty estimates $\delta_{\text{ren}}^{\text{ZEM}_{h1}}$ (left) and $\delta_{\text{ren}}^{\text{OS}_{h2}}$ (right) as function of the DM mass m_A . Note, that the point density is smaller in the right plot as we only consider parameter points, which fulfill the condition $m_{h2} > 2m_A$. We find that in the mass range $m_A \lesssim 450$ GeV, the uncertainty ranges between -25 and $+17\%$. This increases up to 68% with increasing DM masses. Note that we showed in Fig. 17.3 that the relative corrections are large in the large DM mass range. As the difference between the decaying particle h_1 and m_A increases the counterterm δv_S increases. This leads to worse perturbative convergence, which leads to larger theoretical uncertainties due to missing higher-order corrections. On the other hand, a better convergence is found in the OS scheme. As in our parameter scan no large mass gap are possible, the uncertainty estimate $\delta_{\text{ren}}^{\text{OS}_{h2}}$ based on the change to the OS_{h2} scheme is much smaller in range between -1.3 and 3.1% .

m_{h_1}	m_{h_2}	m_A	v_s	α	$v_s^{\text{ZEM}_{h_1}}$	Scheme	$\Omega_{\text{LO}} h^2$	$\Omega_{\text{corr}} h^2$	$\kappa_{\Omega} [\%]$
125.09	180.628	997.005	231.227	-0.1293	226.994	ZEM $_{h_2}$	0.12001	0.1268	5.631
						ZEM $_{h_1}$	0.1119	0.1283	14.6921

Table 17.1.: Input parameters and calculated relic densities of BP1. The parameter v_s is renormalized in the ZEM $_{h_2}$ scheme, while the input parameter $v_s^{\text{ZEM}_{h_1}}$ is obtained via Eq. (15.48). The parameter α is renormalized in the OS scheme.

m_{h_1}	m_{h_2}	m_A	v_s^{OS}	v_s^{p*}	α_{OS}	α_{p*}	Scheme	$\Omega_{\text{LO}} h^2$	$\Omega_{\text{corr}} h^2$	$\kappa_{\Omega} [\%]$
125.09	180.628	997.005	231.227	231.2357	-0.1293	-0.1290	OS	0.12001	0.1268	5.631
							p^*	0.12003	0.12678	5.63071

Table 17.2.: Input parameters and calculated relic densities of benchmark point BP1. The input parameter v_s is renormalized in the ZEM $_{h_2}$ scheme using the OS counterterm $\delta\alpha^{\text{OS}}$. The values v_s^{p*} and α_{p*} are obtained via Eq. (15.48). The relic density is computed once in each scheme.

In this part of the thesis, we investigated the impact of the relic density in the framework of the CxSM, which we introduced in Sec. 2.2. Within the scope of this project, we extended the public code `RelExt` with the calculation of the relic density at next-to-leading order, which we will extend in future work to automate the implementation of higher-order calculations in an arbitrary model.

We have presented how the relic density is obtained at next-to-leading order. In Ch. 15, we demonstrated how we obtain UV- and IR-finite cross sections for our calculation. Afterwards, we presented the applied theoretical and experimental constraints and the scan ranges of our parameter sample. Finally, in Ch. 17, we presented the impact of the higher-order corrections on the dark matter relic abundance. Here, we provided as a proof-of-concept the results first only with next-to-leading order QCD corrections. Next, we presented the electroweak and the QCD corrections and the impact of different renormalization schemes. We have shown that the higher-order corrections can lead to either an increase or a decrease of the relic density. This has an important phenomenological consequence: higher-order corrections can invalidate previously valid parameter points by increasing the relic density such that it exceeds the observed dark matter relic abundance measured by the PLANCK experiment [3]. Vice versa, due to possibly negative higher-order corrections to the relic density, it can occur, that previously discarded parameter points, which oversaturated the relic density, can become valid again. Furthermore, we have shown that the theoretical uncertainty between the renormalization schemes are small if the variation of the input parameters that are affected by the change in scheme is small.

Overall, we have shown that the inclusion of higher-order calculations are important to explore the parameter space of a given dark matter model.

Part V.

Conclusion and Overview

Final Conclusion and Outlook

The success story of the Standard Model of particle physics was further advanced by the discovery of the Higgs boson in 2012. However, despite its many precise predictions, the Standard Model still lacks solutions to some unanswered problems. In this thesis, we focused on understanding the nature of dark matter in the universe by investigating various theories beyond the Standard Model. A very important observable is the dark matter relic density $\Omega_c h^2$, which has been measured by the PLANCK collaboration to be

$$\Omega_c h^2 = 0.1200 \pm 0.0012 . \quad (19.1)$$

The computation of the relic density in a theory beyond the Standard Model can become tedious, in particular for more complex models. This task becomes even more difficult when the goal is to find the parameter configuration that yields the correct experimental relic density. To solve this issue, we developed, within the scope of this thesis, the C++ code **RelExt**, which automates the computation of the relic density via freeze-out for an arbitrary model with a dark matter candidate stabilized by a discrete symmetry. Furthermore, we implemented search algorithms that conveniently provide the parameter configurations which yield the experimentally observed relic density. Also, due to its modular structure, the code can easily be extended to implement new features, such as computing the direct-detection cross section or calculating higher-order corrections to the relic density.

In Part I, we briefly introduced the Standard Model, and the beyond-the-Standard Model (BSM) theories investigated in this thesis, which are the Complex Singlet Extension of the Standard Model, the Complex Two-Higgs Doublet Model, and the Next-To Minimal Supersymmetric Standard Model. Afterward, we gave a brief introduction to the Standard Model of Cosmology. Furthermore, we provided derivations of the Boltzmann equation for calculating the dark matter relic density and of the direct detection cross section.

To provide precise theoretical predictions, we need a deeper understanding of the experimental constraints and their interplay within BSM theories. Therefore, in Part II of this thesis, we studied the interplay of collider and electric dipole constraints by investigating the allowed CP-violation of the coupling between a fermion pair and a Standard Model-like Higgs boson. We first introduced expressions for calculating the electric dipole moment, including kite diagrams, which were not included in previous works, followed by a description of the

theoretical and experimental constraints used in our parameter scan. In Ch. 6, we presented the results using traditional scan methods, i.e., using a guided scan method. To potentially reveal previously overlooked regions in the parameter space, we employed machine learning algorithms, specifically the CMA-ES algorithm, to explore it. In Ch. 7, we provided a short description of the machine learning algorithm, as well as the presentation of our results.

Exploring the parameter space of the Next-to-Minimal Supersymmetric Standard Model is a complicated and computationally intensive task. To circumvent this issue, we presented in Part III our new tool **NMSSMScanner**, which provides a convenient way to explore the parameter space of the Next-to-Minimal Supersymmetric Standard Model. In Ch. 9, we presented the theoretical framework necessary for the evaluation of the relic density and the direct detection cross section in this model. Within the scope of this work, **RelExt**, introduced in Ch. 10, was extended to include the calculation of these dark matter observables. Afterward, we provided an overview of the tool **NMSSMScanner**, presenting the experimental and theoretical constraints, as well as the computer codes used in the program chain. As a proof-of-concept of this tool, we maximized the production cross section of a resonant non-Standard Model Higgs boson into various final states, as well as investigating the dark matter observables in the Next-to Minimal Supersymmetric Standard Model. A detailed description of our results is given in Ch. 12.

In the final Part IV of this thesis, we computed the dark matter relic abundance at next-to-leading order electroweak and QCD in the framework of the Complex Singlet Extension of the Standard Model. In order to do so, we implemented the next-to-leading order annihilation amplitudes squared in **RelExt**. In Ch. 15, we presented the prescriptions needed in order to obtain UV- and IR-finite annihilation cross sections. Afterward, we presented the applied theoretical and experimental constraints, as well as the scan ranges used in the investigated parameter sample. In Ch. 17, we showed the impact of higher-order corrections on the relic density, as well as the phenomenological consequences of these, where we saw that the higher-order corrections can both increase or decrease the computed relic density, making the higher-order calculation an important contribution to future studies of the validity of parameter points.

Even though the Standard Model is a success story in itself, the unanswered questions show us that there is still new physics to be discovered. In order to do so, we need precise calculations within the Standard Model as well as in theories beyond the Standard Model. In particular, there is a lack of precision in calculations in dark matter models. However, experiments for dark matter searches become increasingly precise. Therefore, the need for precise theoretical predictions becomes increasingly relevant to solving the mystery of dark matter in the universe. With this thesis, we provided a contribution to further proceed on this path.

Relevant Couplings for the Direct Detection Calculation in the NMSSM

We will provide the relevant couplings required to compute the DD cross-section in the NMSSM. Here, we will follow the description given in Ref. [135].

A.1. Higgs-Quark-Quark Interaction

The Lagrangian $\mathcal{L}_{qqh}$, which parametrizes the interaction between the CP-even Higgs mass eigenstates h_a^0 ($i \in [1, 2, 3]$) and the quarks can be denoted as

$$\mathcal{L}_{qqh} = -\bar{q}_i [C_{YL}^i P_L + C_{YR}^i P_R] q_i h_a^0. \quad (\text{A.1})$$

Here, the index denotes the up-type $i = 1$ and the down-type quark $i = 2$. Further, we have omitted the quark generation indices. The couplings C_{YL}^i and C_{YR}^i read

$$C_{YL}^i = C_{YR}^i = C_Y^i; \quad C_Y^1 = -\frac{g_2 m_u}{2m_W \sin \beta} \mathcal{R}'_{a2}, \quad C_Y^2 = \frac{g_2 m_d}{2m_W \cos \beta} \mathcal{R}'_{a1}, \quad (\text{A.2})$$

where $\mathcal{R}' \equiv \mathcal{R} \mathcal{R}_G$ and $\mathcal{R}$ and $\mathcal{R}_G$ are defined in Eqs. (??) and (2.86).

A.2. Neutralino-Neutralino-Higgs Interaction

The Lagrangian $\mathcal{L}_{h\tilde{\chi}^0\tilde{\chi}^0}$, which describes the interaction between the CP-even Higgs mass eigenstates h_a^0 ($a \in [1, 2, 3]$) and the two neutralinos $\tilde{\chi}_\alpha^0$ and $\tilde{\chi}_\beta^0$ ($\alpha, \beta \in [1, 2, 3, 4, 5]$) is written as

$$\mathcal{L}_{h\tilde{\chi}^0\tilde{\chi}^0} = \frac{1}{4} h_a^0 \tilde{\chi}_\alpha^0 [C_{HL}^{a,\alpha\beta} P_L + C_{HR}^{a,\alpha\beta} P_R] \tilde{\chi}_\beta^0. \quad (\text{A.3})$$

The coupling $C_{HL}^{a,\alpha\beta}$ is given by

$$\begin{aligned} C_{HL}^{a,\alpha\beta} = & [-g_2 (\mathcal{N}_{\alpha 2}^* - \tan \theta_W \mathcal{N}_{\alpha 1}^*) (\mathcal{R}'_{a1} \mathcal{N}_{\beta 3}^* - \mathcal{R}'_{a2} \mathcal{N}_{\beta 4}^*) \\ & + \sqrt{2} \lambda [\mathcal{R}'_{a3} \mathcal{N}_{\alpha 3}^* \mathcal{N}_{\beta 4}^* + \mathcal{N}_{\beta 5}^* (\mathcal{R}'_{a2} \mathcal{N}_{\alpha 3}^* + \mathcal{R}'_{a1} \mathcal{N}_{\alpha 4}^*) + (\alpha\beta)] \\ & - 2\sqrt{2} \kappa \mathcal{R}'_{a3} \mathcal{N}_{\alpha 5}^* \mathcal{N}_{\beta 5}^*], \end{aligned} \quad (\text{A.4})$$

and $C_{HR}^{a,\alpha\beta}$ reads

$$C_{HR}^{a,\alpha\beta} = (C_{HL}^{a,\alpha\beta})^*. \quad (\text{A.5})$$

In the calculation of the direct detection in Part III, we only consider the Higgs interaction with the lightest neutralino, i.e. $\alpha = \beta = 1$, such that we set $C_{HL}^a \equiv C_{HL}^{a11}$ and $C_{HR}^a \equiv C_{HR}^{a11}$.

A.3. Neutralino-Squark-Quark Interaction

The Lagrangian $\mathcal{L}_{q\tilde{q}\tilde{\chi}^0}$, which describes the interaction between a quark q_i , squark $\tilde{q}_i$ ($i \in [1, 2]$) and neutralino $\tilde{\chi}_\alpha^0$ ($\alpha \in [1, 2, 3, 4, 5]$) reads

$$\mathcal{L}_{q\tilde{q}\tilde{\chi}^0} = \bar{q}_i [C_L^{\alpha Xi} P_L + C_R^{\alpha Xi} P_R] \tilde{\chi}_\alpha^0 \tilde{q}_i^X \quad (\text{A.6})$$

Here, the subscript i denotes the up- ($i = 1$) and down- ($i = 2$) type quarks and squarks, the superscript $X \in \{1, 2\}$ denote the squark mass eigenstates. Again, we are not showing the quark and squark generation indices for readability.

The squark mass eigenstates $\tilde{q}_i$ are related to the chiral eigenstates $\tilde{q}_L$ and $\tilde{q}_R$ via the following rotation

$$\begin{pmatrix} \tilde{q}_1 \\ \tilde{q}_2 \end{pmatrix} = \begin{pmatrix} \eta_{11}^{\tilde{q}} & \eta_{12}^{\tilde{q}} \\ \eta_{12}^{\tilde{q}} & \eta_{22}^{\tilde{q}} \end{pmatrix} \begin{pmatrix} \tilde{q}_L \\ \tilde{q}_R \end{pmatrix}. \quad (\text{A.7})$$

Here, the matrix elements of the rotation matrix are given by $\eta_{11}^{\tilde{q}} = \eta_{22}^{\tilde{q}} = \cos \theta_{\tilde{q}}$ and $\eta_{12}^{\tilde{q}} = -\eta_{21}^{\tilde{q}} = \sin \theta_{\tilde{q}}$. The couplings for the up-type quark and squarks read

$$C_L^{\alpha 11} = -\sqrt{2}g_2 \left[\frac{Y_u}{2} \tan \theta_W \mathcal{N}_{\alpha 1}^* \sin \theta_{\tilde{u}} + \frac{m_u}{2m_W \sin \beta} \mathcal{N}_{\alpha 4}^* \cos \theta_{\tilde{u}} \right], \quad (\text{A.8})$$

$$C_R^{\alpha 11} = -\sqrt{2}g_2 \left\{ \left[\mathcal{N}_{\alpha 2}^* T_3^u + \frac{Y_Q}{2} \tan \theta_W \mathcal{N}_{\alpha 1}^* \right] \cos \theta_{\tilde{u}} + \frac{m_u}{2m_W \sin \beta} \mathcal{N}_{\alpha 4}^* \sin \theta_{\tilde{u}} \right\}, \quad (\text{A.9})$$

$$C_L^{\alpha 21} = -\sqrt{2}g_2 \left[\frac{Y_u}{2} \tan \theta_W \mathcal{N}_{\alpha 1}^* \cos \theta_{\tilde{u}} - \frac{m_u}{2m_W \sin \beta} \mathcal{N}_{\alpha 4}^* \sin \theta_{\tilde{u}} \right], \quad (\text{A.10})$$

$$C_R^{\alpha 21} = -\sqrt{2}g_2 \left\{ \left[-\mathcal{N}_{\alpha 2}^* T_3^u + \frac{Y_Q}{2} \tan \theta_W \mathcal{N}_{\alpha 1}^* \right] \sin \theta_{\tilde{u}} + \frac{m_u}{2m_W \sin \beta} \mathcal{N}_{\alpha 4}^* \cos \theta_{\tilde{u}} \right\}. \quad (\text{A.11})$$

Here, Y_i ($i \in [u, Q]$) denotes the hypercharge of the $SU(2)_L$ of the quark doublet ($i = Q$) or the up-type singlet $i = u$, T_3^u denotes the isospin of the left-handed up-type field u_L . The couplings for the down-type quark are obtained by the following replacements:

$$Y_u \rightarrow Y_d, \quad T_3^u \rightarrow T_3^d, \quad m_u \rightarrow m_d, \quad \theta_{\tilde{u}} \rightarrow \theta_{\tilde{d}}, \quad \sin \beta \rightarrow \cos \beta, \quad \mathcal{N}_{\alpha 4} \rightarrow \mathcal{N}_{\alpha 3}. \quad (\text{A.12})$$

As we are only interested in the interaction between the lightest neutralino $\tilde{\chi}_1^0$, i.e. $\alpha = 1$, and a squark quark pair, we used the following notation $C_{L,R}^{1Xi} \equiv C_{L,R}^{Xi}$

RelExt - Overview on the Mathematica Code and Direct Detection Class

B.1. Mathematica Code

In this section, we provide a more detailed description of the `Mathematica` code implemented in `RelExt`. Here, we will follow the description in Ref. [129].

The implementation of a new model in `RelExt` is fully automated. Here, the implementation involves two `Mathematica` scripts, which are saved in the directory `mathematica`. The first script `FR_to_CH_FA.m` automatically converts the `FeynRules` model file into `FeynArts` (FA) and `CalcHep` (CH) files. The generated files can then be found in the folders `FA_modfiles` and `CH_modfiles`. These folders are localized in the `$RelExt/md_[ModelName]/FR_modfiles/` directory.²⁶ The second `Mathematica` script, `amp2cpp.m`, generates and stores all amplitudes needed to compute the Freeze-Out relic abundance for a DM particle, as well as all information required to implement a new model. This script can be divided into three different building blocks: the amplitude generation block, the decay width generation block and the conversion from `Mathematica` to C++ code block. In the following, we provide an overview of the most important functions, lists, and segments for each block.

The most important elements of the amplitude generation block are

- `particlelist` is a list, where the FA particle identifiers, their masses, the names and PDG numbers are stored. Here, we also include anti-particles; however, exclude Goldstone bosons and ghost particles.
- The function `determineDof[pID_]` determines the degrees of freedom of the particle, which is given by the FA identifier `pID_`.
- The lists `dslist`(FA particle identifier), `dsmass`(mass), `dsnames`(name) and `dsDof`(degrees of freedom) store the information of the dark sector particles. The corresponding information are given in the brackets.

²⁶ `$RelExt` denotes the path, where `RelExt` is installed, and `ModelName` is a placeholder name for the name of the user's model.

- `alldiags` provides all tree-level $2 \rightarrow 2$ Feynman diagrams, with two dark sector particles in the initial states and none in the final state.
- The function `removeDuplicate[]` is used to remove redundant processes from the `diagsgrouped` list. Here, a new list `listofprocs` is generated, which is the final list containing all processes necessary for computing the relic abundance. This includes all channels with two dark sector particles in the initial state and none in the final state. In the case of co-annihilation, this leads to redundancy, as channels with the same final state but with an initial state where the particles are swapped also contribute to the relic density. The amplitude, however, is analytically the same. Therefore, we compute only one amplitude, and remove the other one from the list `listofprocs`. The same reasoning applies to processes whose initial state is the charge conjugate of a previous one. To still obtain the correct relic density, we apply a multiplicative factor to the Boltzmann equation to compensate for the removed channels.
- In order to identify all couplings or coupling combinations in the amplitudes, we implemented the function `breakdownAmp[process_,amp_]`, where the input parameters are a list element `process_` of the list `listofprocs` and the amplitude `amp_`. To reduce computation time in the relic density calculation, these expressions are stored as tokens.
- In order to compute the amplitudes for each process in `listofprocs`, we implemented the function `calcAmps[]` in our script. The generated amplitudes are stored in the list `ampslist` and the relevant Freeze-Out processes in the list `foutlist`. We use the lists `coefficientlist`, `mandellist`, and `tokens` in this routine to tokenize the squared amplitude. Further, we save the masses of the participating particles in the lists `mi`, `mj`, `mk` and `ml`.
- We identify the s -channel contributions in the amplitudes with the function `checkdenpol[amp_]`, where the input is a list element of `mandellist`. If a s -channel is found, we transform the denominator of the respective amplitude as described in Sec. 10.1, with the function `addwidthsub[den_]`, where the input is the denominator of the amplitude `amp_` as a string.
- The masses and the total decay widths of the s -channel mediators are stored in the list `relevantWs`.
- For each list element in `foutlist`, the amplitudes squared are generated with the function `calcAmp2s[]`. Each expression is stored in the list `final`. Note, that the compilation of this function can take several minutes, depending on the number of list elements in `foutlist`.

The second block is the width generation block. This block is similar to the previous block, with one main difference. If the found mediator particle is a scalar or pseudoscalar, we do not calculate the total width of this particle with `FeynCalc`, but instead with the procedure provided in Sec. 10.1. The functions and lists used in this block are

- The FA particle identifiers and the decay widths of the s -channel mediators are stored in the lists `relevantWsfield` and `relevantWidth`, respectively. Note that the total decay width of the SM gauge bosons is taken from the input model files.

- All relevant decay processes for the computation of the total width are stored in `foutlistDecays`. Here, we save the FA particle identifier in each column, with the first column denoting the decaying particle and the other two the final-state particles.
- We identify the type of the participating particles in the decay with the function `determineType[sts_,ind_]`. The inputs are any row of the list `foutDecayslist` `sts_` and the corresponding column number `int_`.
- The generated squared amplitudes for the decays and their decay widths are stored in the lists `finalDecays` and `finalDecaysWidth`, respectively.

The last block is the **Mathematica** to **C++** conversion part. Here, the previously obtained expressions for the (co-)annihilation amplitudes squared, the partial decay widths and the relevant informations of the models are converted into **C++** files. This block consists of the following functions and lists

- The list `inifunc[i]` is used to store for each unique channel that contributes to the computation of the relic abundance, the `processname`, the mass, the FA identifier, and the tokenized amplitudes squared. The input parameter `i` is an integer and goes from 1 to the total number of different initial states.
- `external` and `internal` are lists that store all external and internal variables of the model and their definitions, respectively.
- The list `neutralsmasses` stores all the masses of the neutral dark sector particles.
- `processnameDecays` and `possibleiniDecays` are auxiliary lists that store the names of the decay processes and the corresponding decaying particles, respectively.
- `inifuncDecays[i]` is analogous to `inifunc[i]` but is used for decay processes. In addition, it contains two extra columns corresponding to the `couplings` and `particleType` lists.
- `runMasses` contains the masses of the strange, charm, bottom, and top quarks.
- `model.hpp`, `model.cpp`, `init.cpp`, `parametermap.cpp`, `loadparameters.cpp`, and `loadtokens.cpp` contain the declarations and initialization routines for all external and internal model parameters, tokens, amplitudes squared, partial and total decay widths, dark-sector masses, and the masses and widths of the relevant *s*-channel propagators. The file `model.hpp` is located in `$RelExt/md_[ModelName]/`, while all remaining files are stored in `$RelExt/md_[ModelName]/sources/`. If external parameters depend on the running quark masses contained in `runMasses`, they must be redefined in `loadparameters.cpp` such that their values are updated whenever the renormalization scale of the running masses changes. The only exception is the top quark, for which the user-defined pole mass is used.
- `calcwidths.cpp` contains the routines for computing the running quark masses at a given energy scale as well as the total widths of the relevant *s*-channel mediators. For decay processes, the running masses are evaluated at a scale equal to the pole mass of the decaying particle, whereas for DM (co-)annihilation processes, the scale is chosen as twice the DM mass.
- `all[possibleini].cpp` contains the expressions for the amplitudes squared of all DM (co-)annihilation channels associated with a given initial state `[possibleini]`. These files are located in `$RelExt/md_[ModelName]/sources/amp2s`, with separate files for different initial states.

- `[possibleini]flux.cpp` contains the amplitudes squared multiplied by the corresponding flux factors, where the latter are defined in `$RelExt/sources/utls.cpp`. An additional multiplicative factor, `symfac`, may be included to account for equivalent processes removed by the `removeDuplicate[]` routine. These files are stored in `$RelExt/md_[ModelName]/sources/amp2s`.
- `totalW[possibleini]Decays.cpp` contains the expressions for the partial decay widths of the relevant s -channel mediators, where `[possibleini]Decays` denotes the decaying particle. The files are located in `$RelExt/md_[ModelName]/sources/amp2s`, with one file per mediator. For scalar and pseudoscalar particles, hard-coded `partial_width` functions are employed. These functions take as input the particle types in the final state, their masses, and the couplings extracted from the amplitudes squared, as described in Sec. 10.1. For all other particle types, the decay widths are computed using `FeynCalc`. Off-shell decay channels are assigned a width of zero.
- `prtcls.cpp` contains the definitions of all particle and anti-particle names used in the model. Particles that are their own anti-particles are listed only once.

B.2. Direct Detection Class

In Tab. B.1, we present all functions of the implemented in the class `DDetection`, which is responsible for calculating the spin-independent direct detection cross-section. In the `maincl.hpp`, the `DDetection` class can be found and reads as

```

1   class DDetection {
2   public:
3       DDetection(double m_chi, double Z, double A);
4       void setLambda(const std::string &key, double value);
5       double DDxSecp();
6       double DDxSecn();
7       static double computeMu(double m_chi);
8       void checkRequiredInputs() const;
9       template <typename K, typename V>
10      V safeAt(const std::map<K, V> &m, const K &key,
11              const std::string &context = "") const;
12      static double convertGeV2ToPicobarn(double sigma_gev2);
13      ~DDetection() {};
14
15  private:
16      double mu_chi, Z, A;
17      std::map<std::string, double> lambda;
18      std::map<std::string, double> fq_p = {
19          {"u", 0.01513}, {"d", 0.0191}, {"s", 0.0447}};
20      std::map<std::string, double> fq_n = {
21          {"u", 0.011}, {"d", 0.0273}, {"s", 0.0447}};
22      double computePart(bool isProton);
23      double getMass(const std::string &q) const;
24  };

```

Function	Description
<code>DDetection(m_chi, Z, A)</code>	Constructor function to initialize an object DDetection . The inputs are the dark matter mass <code>m_chi</code> , the proton number <code>Z</code> , and the atomic number <code>A</code> , which initialize the corresponding class variables with the same name.
<code>setLambda(key, value)</code>	Function to assign the Wilson coefficients value <code>value</code> of the corresponding quark <code>key</code> .
<code>DDxSecp()</code>	Returns the SI-DD cross section for a proton according Eq. (3.85).
<code>DDxSecn()</code>	Returns the SI-DD cross section for a neutron according Eq. (3.85).
<code>computeMu(m_chi)</code>	Returns the reduced mass with the dark matter mass <code>m_chi</code> as input.
<code>safeAt()</code>	This function accesses the value associated with a given key from a map. If the key is not present, it returns an error specifying the missing key and the corresponding context.
<code>convertGeV2ToPicobarn(sigma_gev2)</code>	Returns the spin-independent direct-detection cross section in pb and takes as input the spin-independent direct-detection cross section in GeV^{-2} .
<code>computePart(isProton)</code>	Computes and returns the Wilson coefficient $c_{s,N}$ according to Eq. (3.79). The boolean input parameter <code>isProton</code> checks whether the nucleon is a proton or a neutron.
<code>getMass(q)</code>	Returns the mass of the quark <code>q</code> .

Table B.1.: Descriptions of the functions in the **DDetection** class in order to calculate the spin-independent direct-detection cross section.

APPENDIX C

Benchmark Points used in the Analysis of Part III.

We will provide the benchmark points used in our analysis in Part III. These benchmark points have been taken from Ref. [128].

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.47	0.56	294	-973	212	3.21
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
618.3	825.2	519.1	1350.5	-3358.7	-1372.7
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
923.6	2619.9	3629.3	3847.5	2693.8	2361.8

Table C.1.: BPs4b: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 3.8$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 3$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
62.7	124.6	624.3	617.1	836.7	618.3
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
2.50e-04	4.18e-03	3.97	4.99	6.30	4.12
$\sigma_{H_3}^{\text{NNLO}}$ [fb]	$\text{BR}_{H_3 \rightarrow H_1 H_2}$	$\text{BR}_{H_1 \rightarrow b\bar{b}}$	$\text{BR}_{H_2 \rightarrow b\bar{b}}$	$\sigma_{H_1 H_2}$ [fb]	σ_{max}^s [fb]
144	0.336	0.909	0.617	48.493	27

Table C.2.: BPs4b: The Higgs boson spectrum (upper row) with the total widths (middle row); the NNLO QCD H_3 production cross section, relevant branching ratios, the $H_1 H_2$ and the $4b$ final state cross section values (lower row). The H_1 and A_2 are singlet-like.

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.55	0.36	328	-772	320	1.64
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
605.3	1354.8	539.9	3769.5	-2982.7	-1000.9
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
2248.3	2739.9	2176.4	1996.7	3929.5	1538.2

Table C.3.: BPs2b2gam: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 2.7$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 4$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
125.0	133.1	611.1	605.4	701.0	605.3
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
4.18×10^{-3}	4.66×10^{-5}	8.54	11.43	3.23	10.69
$\sigma_{H_3}^{\text{NNLO}}$ [fb]	$\text{BR}_{H_3 \rightarrow H_1 H_2}$	$\text{BR}_{H_1 \rightarrow b\bar{b}}$	$\text{BR}_{H_2 \rightarrow \gamma\gamma}$	$\sigma_{H_1 H_2}$ [fb]	σ_{max}^s [fb]
617	0.041	0.613	7.787×10^{-3}	25.025	0.119

Table C.4.: BPs2b2gam: The Higgs boson spectrum (upper row) with the total widths (middle row); the NNLO QCD H_3 production cross section, relevant branching ratios, the $H_1 H_2$ and the $(2b)(2\gamma)$ final state cross section values (lower row). The H_2 and A_2 are singlet-like.

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.49	0.58	258	-1054	229	2.78
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
601.0	951.8	476.9	1404.4	-3456.2	-1189.7
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
1045.8	2378.6	3732.3	3879.7	2601.3	2249.4

Table C.5.: BPs2gam2b: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 3.8$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 3.1$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
81.1	126.7	608.0	599.9	907.1	601.0
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
6.65e-04	3.79e-03	4.33	5.88	7.59	4.87
$\sigma_{H_3}^{\text{NNLO}}$ [fb]	$\text{BR}_{H_3 \rightarrow H_1 H_2}$	$\text{BR}_{H_1 \rightarrow b\bar{b}}$	$\text{BR}_{H_2 \rightarrow \gamma\gamma}$	$\sigma_{H_1 H_2}$ [fb]	σ_{max}^s [fb]
219	0.228	0.903	2.673×10^{-3}	50.0	0.121

Table C.6.: BPs2gam2b: The Higgs boson spectrum (upper row) with the total widths (middle row); the NNLO QCD H_3 production cross section, relevant branching ratios, the $H_1 H_2$ and the $(2\gamma)(2b)$ final state cross section values (lower row). The H_1 and A_2 are singlet-like.

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.56	0.57	106	-65	346	1.80
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
603.2	894.8	1284.0	3177.1	-3598.7	3886.4
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
1582.9	1306.4	1766.9	3700.3	3060.5	2323.5

Table C.7.: BPP4b: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 2.6$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 3.4$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
125.7	594.4	690.0	273.1	614.2	603.2
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
4.25^{-3}	7.05	3.62	7.26^{-4}	9.93	9.71
$\sigma_{A_2}^{\text{NNLO}}$ [fb]	$\text{BR}_{A_2 \rightarrow H_1 A_1}$	$\text{BR}_{H_1 \rightarrow b\bar{b}}$	$\text{BR}_{H_1 \rightarrow \tau\bar{\tau}}$	$\text{BR}_{A_1 \rightarrow b\bar{b}}$	$\sigma_{H_1 A_1}$ [fb]
772	0.123	0.596	0.064	0.737	94.588

Table C.8.: BPP4b: The Higgs boson spectrum (upper row) with the total widths (middle row); the NNLO QCD A_2 production cross section, relevant branching ratios (for the $4b$ and $(\tau\bar{\tau})(b\bar{b})$ final states) and the $H_1 A_1$ section value (lower row). Further relevant branching ratios for the $(\gamma\gamma)(b\bar{b})$ and $(\gamma\gamma)(\tau\bar{\tau})$ final states are $\text{BR}_{H_1 \rightarrow \gamma\gamma} = 2.32 \times 10^{-3}$ and $\text{BR}_{A_1 \rightarrow \tau\tau} = 0.091$. The H_3 and A_1 are singlet-like.

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.58	0.58	243	-38	330	1.19
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
601.6	419.3	1104.4	3209.0	-3541.2	3769.5
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
1473.0	1370.4	1762.2	3946.3	3173.3	2254.4

Table C.9.: BPP2b2gam: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 2.5$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 3.4$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
124.9	602.4	638.8	243.2	608.1	601.6
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
4.13×10^{-3}	14.67	4.62	1.83×10^{-4}	20.73	19.96
$\sigma_{A_2}^{\text{NNLO}}$ [fb]	$\text{BR}_{A_2 \rightarrow H_1 A_1}$	$\text{BR}_{H_1 \rightarrow b\bar{b}}$	$\text{BR}_{H_1 \rightarrow \tau\bar{\tau}}$	$\text{BR}_{A_1 \rightarrow \gamma\gamma}$	$\sigma_{H_1 A_1}$ [fb]
1889	0.034	0.612	0.066	9.0×10^{-3}	64.325

Table C.10.: BPp2b2gam: The Higgs boson spectrum (upper row) with the total widths (middle row); the NNLO QCD A_2 production cross section, relevant branching ratios and the $H_1 A_1$ cross section value (lower row). The H_3 and A_1 are singlet-like.

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.55	0.50	318	-983	432	1.96
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
846.3	1050.2	1676.9	3188.2	-2592.8	3316.8
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
2208.9	3574.2	3712.5	-2193.5	3907.3	3766.5

Table C.11.: BPps2b2t: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 3.1$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 2.5$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
124.1	459.9	852.3	844.2	1056.5	846.3
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
3.98×10^{-3}	0.03	40.44	11.28	7.89	11.10
$\sigma_{H_3}^{\text{NNLO}}$ [fb]	$\text{BR}_{H_3 \rightarrow H_1 H_2}$	$\text{BR}_{H_1 \rightarrow b\bar{b}}$	$\text{BR}_{H_2 \rightarrow t\bar{t}}$	$\sigma_{H_1 H_2}$ [fb]	σ_{max}^s [fb]
71	0.768	0.614	0.903	54.375	30

Table C.12.: BPps2b2t: The Higgs boson spectrum (upper row) with the total widths (middle row); the NNLO QCD H_3 production cross section, relevant branching ratios, the $H_1 H_2$ cross and the $(b\bar{b})(t\bar{t})$ final state cross section values (lower row). The H_2 and A_2 are singlet-like.

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.59	0.60	62	-151	344	2.43
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
610.5	1491.1	502.4	2709.1	-3223.0	-1672.9
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
2940.3	2676.9	1908.6	2158.1	3759.3	1650.9

Table C.13.: BPp2b2t: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 2.7$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 3.9$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
123.9	583.1	667.2	380.8	626.4	610.5
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
3.92×10^{-3}	2.47	2.74	0.16	5.75	5.77
$\sigma_{A_2}^{\text{NNLO}}$ [fb]	$\text{BR}_{A_2 \rightarrow H_1 A_1}$	$\text{BR}_{H_1 \rightarrow b\bar{b}}$	$\text{BR}_{A_1 \rightarrow t\bar{t}}$	$\sigma_{H_1 A_1}$ [fb]	σ_{max}^p [fb]
371	0.165	0.614	0.977	61.290	37

Table C.14.: BPp2b2t: The Higgs boson spectrum (upper row) with the total widths (middle row); the NNLO QCD A_2 production cross section, relevant branching ratios, the $H_1 A_1$ and the $(b\bar{b})(t\bar{t})$ cross section values (lower row). The H_3 and A_1 are singlet-like.

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.57	0.60	93	-1146	332	2.11
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
601.0	416.4	530.9	3619.6	-3830.3	-1757.8
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
3220.0	3868.4	2756.0	1707.5	3168.4	1937.6

Table C.15.: BPs6b: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 2.9$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 3.6$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
124.0	291.5	610.4	599.0	1059.3	601.0
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
3.82e-03	0.15	5.54	7.32	12.51	6.97
$\sigma_{H_3}^{\text{NNLO}}$ [fb]	$\text{BR}_{H_3 \rightarrow H_1 H_2}$	$\text{BR}_{H_1 \rightarrow b\bar{b}}$	$\text{BR}_{H_2 \rightarrow b\bar{b}}$	$\text{BR}_{H_2 \rightarrow H_1 H_1}$	$\sigma_{H_1 H_2}$ [fb]
374	0.110	0.608	0.006	0.435	41.214

Table C.16.: BPs6b: The Higgs spectrum (upper row) with the total widths (middle row); the NNLO QCD H_3 production cross section, relevant branching ratios and the resulting $H_1 H_2$ cross-section (lower row). The H_1 and A_2 are singlet-like.

λ	κ	A_λ [GeV]	A_κ [GeV]	μ_{eff} [GeV]	$\tan \beta$
0.63	0.51	234	-931	326	1.86
$m_{H^\pm}$ [GeV]	M_1 [GeV]	M_2 [GeV]	M_3 [GeV]	A_t [GeV]	A_b [GeV]
601.8	1367.0	553.8	3625.9	-3011.3	-1105.9
$m_{\tilde{Q}_3}$ [GeV]	$m_{\tilde{t}_R}$ [GeV]	$m_{\tilde{b}_R}$ [GeV]	A_τ [GeV]	$m_{\tilde{L}_3}$ [GeV]	$m_{\tilde{\tau}_R}$ [GeV]
2202.1	2844.5	2240.8	2224.3	3812.2	1446.5

Table C.17.: BPs2gamma2w: NMSSM input parameters. The soft breaking masses of the first two generations are $m_{\tilde{Q}_{1,2}} = m_{\tilde{L}_{1,2}} = 2.55$ TeV, $m_{\tilde{u}_R, \tilde{d}_R} = m_{\tilde{c}_R, \tilde{s}_R} = m_{\tilde{e}_R, \tilde{\mu}_R} = 4.0$ TeV.

m_{H_1} [GeV]	m_{H_2} [GeV]	m_{H_3} [GeV]	m_{A_1} [GeV]	m_{A_2} [GeV]	$m_{H^\pm}$ [GeV]
125.6	178.6	610.1	602.5	844.1	601.8
$\Gamma_{H_1}^{\text{tot}}$ [GeV]	$\Gamma_{H_2}^{\text{tot}}$ [GeV]	$\Gamma_{H_3}^{\text{tot}}$ [GeV]	$\Gamma_{A_1}^{\text{tot}}$ [GeV]	$\Gamma_{A_2}^{\text{tot}}$ [GeV]	$\Gamma_{H^\pm}^{\text{tot}}$ [GeV]
3.45×10^{-3}	5.72×10^{-2}	6.98	9.14	7.83	8.78
$\sigma_{H_3}^{\text{NNLO}}$ [fb]	$\text{BR}_{H_3 \rightarrow H_1 H_2}$	$\text{BR}_{H_1 \rightarrow \gamma\gamma}$	$\text{BR}_{H_2 \rightarrow WW}$	$\sigma_{H_1 H_2}$ [fb]	σ_{max}^s [fb]
479	8.69×10^{-2}	2.68×10^{-3}	0.93	41.625	0.104

Table C.18.: BPs2gamma2w: The Higgs boson spectrum (upper row) with the total widths (middle row); the NNLO QCD H_3 production cross section, relevant branching ratios, the $H_1 H_2$ and the $(2\gamma)(2W)$ final state cross section values (lower row). The H_2 and A_2 are singlet-like.

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