Beyond the Standard Model Orders of Charge–Parity Violation

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Summary

The Standard Model (SM) of particle physics is an extremely successful theory, making accurate predictions across many orders of magnitude in agreement with experiments. However, there exists solid evidence that the SM is not a complete description of Nature, calling for physics beyond the SM (BSM). Due to the absence of direct signals of new physics states in experiments in recent years, evidence is growing that BSM physics is either very heavy or light and weakly coupled. In this thesis, we will use effective field theories (EFTs), which are well-suited to describe the effects of heavy particles at low energies.

In Part I, we study CP violation in the SM and SMEFT extended with light sterile neutrinos. We construct the generating set of flavour invariants in the νSM that allows us to express any observable as a polynomial of those invariants. This is in particular useful to study CP violation, as the invariants allow us to express the necessary and sufficient conditions for CP violation in a flavour basis-invariant way. Then, we extend the results to the EFT interactions, where we study different scenarios for the generation of neutrino masses. We find that the form of the EFT flavour invariants and their suppression with the scale of new physics changes drastically depending on the nature of the neutrino masses.

In Part II, we study different aspects of symmetry breaking in the EFTs of axionlike particles (ALPs). An essential property of ALPs is their shift symmetry rooted in their pseudo-Nambu–Goldstone nature. We study the implications of imposing this symmetry in the leading order effective Lagrangian by reformulating well-known matrix relations, that enforce the symmetry in the leading order EFT couplings, into flavour-invariant order parameters of shift symmetry, which allow us to properly impose the power counting of the theory in the presence of a softly broken shift symmetry, which is otherwise not possible.

Using the Hilbert series, we count the number of operators appearing in the ALP EFT with and without a shift symmetry above and below the electroweak scale. We use this information to construct operator bases for the EFTs, generalise the matrix relations imposing shift symmetry to higher order and construct the leading order CP-odd flavour invariants.

The axion solution to the strong CP problem can be spoiled by new sources of CP violation in the ultraviolet in the presence of small instantons. Parameterising new sources of CP violation in the SMEFT, we construct CP-odd SMEFT flavour invariants featuring the strong vacuum angle, necessarily appearing in instanton computations. We show that the invariants explicitly appear in the instanton computations and vice-versa that they can be used to systematise the computations. Using these results, we derive bounds on different small instanton and SMEFT flavour scenarios.

Zusammenfassung

Das Standardmodell (SM) der Teilchenphysik ist eine äußerst erfolgreiche Theorie, die über viele Größenordnungen hinweg genaue Vorhersagen in Übereinstimmung mit Experimenten macht. Es gibt jedoch stichhaltige Beweise dafür, dass das SM keine vollständige Beschreibung der Natur ist, was Physik jenseits des SM erfordert. Da in den letzten Jahren keine direkten Signale für Zustände neuer Physik in Experimenten gefunden wurden, mehren sich die Hinweise, dass die Physik jenseits des SM entweder sehr schwer oder leicht und schwach gekoppelt sein muss. In dieser Arbeit werden wir effektive Feldtheorien (EFTs) verwenden, die gut geeignet sind, die Effekte schwerer Teilchen bei niedrigen Energien zu beschreiben.

In Teil I untersuchen wir die CP-Verletzung im SM und in der SMEFT erweitert mit leichten sterilen Neutrinos. Wir konstruieren die erzeugende Menge von Flavourinvarianten im νSM, die es uns ermöglicht, jede Observable als Polynom dieser Invarianten auszudrücken. Dies ist insbesondere nützlich um CP-Verletzung zu untersuchen, da die Invarianten es ermöglichen, die notwendigen und hinreichenden Bedingungen für CP-Verletzung flavourbasisinvariant auszudrücken. Anschließend weiten wir die Ergebnisse auf die EFT-Wechselwirkungen aus, wo wir verschiedene Szenarien für die Erzeugung von Neutrinomassen untersuchen. Wir stellen fest, dass sich die Form der EFT-Flavourinvarianten und ihre Unterdrückung mit der Skala der neuen Physik drastisch mit der untersuchten Art der Neutrinomassen ändert.

In Teil II untersuchen wir verschiedene Aspekte der Symmetriebrechung in den EFTs von axionartigen Teilchen (ALPs). Eine wesentliche Eigenschaft von ALPs ist ihre Shiftsymmetrie, die in ihrer Pseudo-Nambu–Goldstone-Natur begründet ist. Wir untersuchen die Auswirkungen dieser Symmetrie auf die führenden effektiven Operatoren, indem wir bekannte Matrixbeziehungen, die eine Shiftsymmetrie für die EFT-Kopplungen erster Ordnung erzwingen, in flavour-invariante Ordnungsparameter der Shiftsymmetrie umformulieren, die ermöglichen das Powercounting der Theorie bei einer leicht gebrochenen Shiftsymmetrie korrekt zu implementieren. Mit Hilfe der Hilbertreihe zählen wir die Anzahl der Operatoren, die in der ALP EFT mit und ohne Shiftsymmetrie oberhalb und unterhalb der elektroschwachen Skala auftreten. Wir nutzen diese Information, um Operatorbasen für die EFTs zu konstruieren, die Matrixbeziehungen, die eine Shiftsymmetrie erzwingen, auf höhere Ordnung zu verallgemeinern und die CP-verletzenden Flavourinvarianten führender Ordnung zu konstruieren.

Die Lösung des starken CP-Problems durch das Axion kann durch neue Quellen der CP-Verletzung im Ultravioletten in Anwesenheit von kleinen Instantonen gestört werden. Nachdem wir neue Quellen der CP-Verletzung in der SMEFT parametrisieren, konstruieren wir CP-verletzende SMEFT-Flavourinvarianten mit dem starken Vakuumwinkel, der notwendigerweise in den Instanton-Berechnungen auftaucht. Wir zeigen, dass die Invarianten explizit in den Instantonberechnungen erscheinen und umgekehrt, dass sie zur Systematisierung der Berechnungen verwendet werden können. Mit den Ergebnissen leiten wir Limits für verschiedene kleine Instanton- und SMEFT-Flavourszenarien ab.

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Declaration of Independent Work

I declare that I have completed the thesis independently using only the aids and tools specified. I have not applied for a doctor's degree in the doctoral subject elsewhere and do not hold a corresponding doctor's degree. I have taken due note of the Faculty of Mathematics and Natural Sciences PhD Regulations, published in the Official Gazette of Humboldt-Universität zu Berlin no. 42/2018 on 11/07/2018.

Hamburg, 15 July 2024 Jonathan Kley

List of Publications

This dissertation is largely based on the following publications and preprint

[1] Q. Bonnefoy, C. Grojean and J. Kley, "Shift-Invariant Orders of an Axionlike Particle", Phys. Rev. Lett. **130**, 111803 (2023), arXiv:2206.04182 [hep-ph].

[2] C. Grojean, J. Kley and C.-Y. Yao, "Hilbert series for ALP EFTs", JHEP **11**, 196 (2023), arXiv:2307.08563 [hep-ph].

[3] R. Bedi, T. Gherghetta, C. Grojean, G. Guedes, J. Kley and P. N. H. Vuong, "Small instanton-induced flavor invariants and the axion potential", JHEP **06**, 156 (2024), arXiv:2402.09361 [hep-ph].

[4] C. Grojean, J. Kley, D. Leflot and C.-Y. Yao, "The flavor invariants of the νSM", (2024), arXiv:2406.00094 [hep-ph], submitted to JHEP, under review.

Chapter 3 contains all the results published in Ref. [4]. Chapter 4 reports on some unpublished work in progress in collaboration with Christophe Grojean and Chang-Yuan Yao, building on the results of Chapter 3. Chapter 6 contains results from Ref. [1]. Chapter 7 contains results from Ref. [2]. Chapter 8 is mostly based on Ref. [3]. In particular, some figures and tables contained in this dissertation have previously appeared in these articles.

In addition, the following publication and preprint not included in this thesis were published during the completion of this PhD project

[5] J. Kley, T. Theil, E. Venturini and A. Weiler, "Electric dipole moments at one-loop in the dimension-6 SMEFT", Eur. Phys. J. C **82**, 926 (2022), arXiv:2109.15085 [hep-ph].

[6] Q. Bonnefoy, J. Kley, D. Liu, A. N. Rossia and C.-Y. Yao, "Aligned Yet Large Dipoles: a SMEFT Study", (2024), arXiv:2403.13065 [hep-ph], submitted to JHEP, under review.

Contents

1 Introduction

Since the early days of humankind, humans have tried to find patterns in their environment striving to understand better the world they live in. From the motion of planets and stars on the night sky and simple mechanical principles to Newtonian gravity and electromagnetism to the understanding of subatomic physics, special relativity and quantum physics, this curiosity has slowly developed into a robust scientific method of modelling phenomena observed in Nature and vigorously testing our current best understanding of those phenomena. In this endeavour, we managed to understand the principles that govern our universe at smaller and smaller scales by reducing the dynamics at the current scale to a minimal model among the relevant degrees of freedom.

At the top of these decades and centuries of research lies the Standard Model (SM) of particle physics, our current best understanding of fundamental physics at the smallest length scales. With the discovery of a 125 GeV boson at the LHC [7, 8] in 2012 all constituents of the Standard Model (SM) [9–20] have been detected in experiment. The model is incredibly successful as it can predict cross sections of scattering experiments across 14 orders of magnitude in agreement with experimental measurements [21]. Its best prediction, the prediction of the anomalous magnetic moment of the electron [22], is in agreement with experiment [23] to an astonishing twelve significant digits. With this outstanding understanding of particle physics on the one side, there are also a handful of phenomena in Nature that cannot be understood within the SM. On the one side, there exist serious problems of the SM, like dark matter, neutrino masses, the matter-antimatter asymmetry and the fundamental quantum theory of gravity, which are all phenomena observed in Nature that cannot be explained within the SM. On the other hand, the Standard Model is also troubled by some aesthetic issues, all boiling down to our lack of understanding the value of certain parameters, which include the strong CP problem and the hierarchy problems.

Hence, new physics beyond the SM (BSM) is needed to explain these discrepancies between the SM and the phenomena we observe in Nature. Inspired by the successful reductionist view, that physics at higher and higher energy scales can be reduced by symmetry and explained by fewer and fewer parameters, the hope for a theory of everything that in the most optimistic case can explain Nature with just a single input parameter has prevailed. In this spirit, many theories have been put forward in the last few decades trying to explain some of the discrepancies of the SM. However, after the discovery of the Higgs boson, no direct observation of new physics states have been made in experiment.

Without a clear sign of new physics effects at particle colliders or other experiments in recent years, it is becoming clear that the mass of any BSM particle is either beyond current direct reach or the particles are light and very weakly coupled. A well-suited consistent approach in the case of heavy new physics are effective field theories (EFTs), where only the light known particles appear as dynamic degrees of freedom. All effects of the heavy particles are captured effectively in the interactions among the light degrees of freedom with generic coefficients. The advantage of this approach is that it is mostly model-independent, where the only assumption lies in the knowledge of all relevant light particles and the symmetries that govern their interactions. This allows for a systematic study of classes of well-motivated ultraviolet (UV) completions without having to specify all the details of the theory. A particularly interesting class of new physics are models providing new sources of charge-parity (CP) violation, which introduces differences between particles and their antiparticles. Finding new physics with a sizeable source of new CP violation would bring us a step closer to understanding the baryon asymmetry, which if generated via baryogenesis in the early universe requires significant violation of CP, beyond the CP violation in the SM, as formulated in the Zakharov conditions [24].

The EFT of the Standard Model, the Standard Model Effective Field Theory (SMEFT), is constructed by combining all SM fields into operators invariant under the Poincaré symmetry and gauge symmetries of the SM. Considering the operators that do not break lepton and baryon number, which are expected to be good symmetries up to very high energy scales, the SMEFT already has 2499 free parameters, out of which 1149 transform under CP and 1350 do not transform under CP, at the leading order. In the light of this enormous number of free parameters it would be useful to have an organising principle of the couplings, which is based on our knowledge of the SM instead of making some assumptions about the UV physics. Since most of the free parameters of the SMEFT are due to the fact that the SM fermions come in 3 generations, one curious observation is that the only flavourful SM couplings, the SM Yukawa couplings are hierarchical with the Yukawa coupling of the electron being $y_e \approx 3 \cdot 10^{-6}$ and the Yukawa coupling of the top being $y_t \approx 1$ [25]. Furthermore, the elements of the mixing matrix in the quark sector of the SM are rather small, yielding a further suppression of flavourful couplings.

Another simple but important observation is that observables should be independent of the mathematical basis chosen to compute them, in particular the flavour basis. Hence, building objects from the Wilson coefficients and the SM Yukawa couplings that are invariant under flavour transformations combined with the suppression of the SM Yukawa couplings could yield a good organising principle for the Wilson coefficients, in particular the CP-odd ones we are interested in. There are several questions that need to be answered: How do the CP-odd flavour invariants of commonly used EFTs look like and how can they be constructed? Are the EFT flavour invariants constructed in this way really the fundamental objects appearing in computations or do they appear enhanced or suppressed by other quantities?

As mentioned previously, there could also exist light new physics that has escaped our experiments up to this point due to their very feeble couplings to the SM particles. Two examples that we consider in this thesis are axions (and axionlike particles (ALPs)) and light sterile neutrinos, which are solutions to the strong CP problem and the non-existence of neutrino masses in the renormalisable SM, respectively. When these particles are added to the spectrum of light particles used to construct the EFT, the number of free parameters usually also increases rapidly with the number of flavours and understanding if heavy physics related to the appearance of these particles at low energies can bring new sources of CP violation is of interest.

One of the defining properties of the axion is its shift symmetry rooted in its pseudo-Nambu–Goldstone nature. In the EFT, this property is usually implemented by only coupling the axion derivatively to other fields. However, in EFTs there exist certain redundancies that allow us to trade derivatives acting on fields by other terms that contain more fields instead of the derivatives. Moreover, in the presence of a soft breaking of the axion shift symmetry also non-derivatively coupled interactions of the axions to other fields have to be added. It then has to be addressed how the shift-preserving and shift-breaking interactions can be disentangled after taking into account the redundancies due to the derivative couplings.

Furthermore, if new sources of CP violation exist in the UV, they can affect the axion solution to the strong CP problem, which is constructed to remove the CP violation present in the Lagrangian describing the strong interactions. Parameterising the new sources of CP violation in the SMEFT, an immediate question is whether the contributions of the CP-violating parameters in the SMEFT come in a flavour-invariant form as conjectured earlier.

In this thesis, we will try to answer these questions. As it will turn out, flavour invariants will play a central role in approaching many of these issues systematically. The thesis is split into two parts. In Part I, we will study CP violation in the SM extended with light sterile neutrinos and its effective theory in the language of flavour invariants. In Part II, we will study different aspects of symmetry breaking in the effective theory of axionlike particles with the help of flavour invariants and the Hilbert series.

In Chap. 2, we introduce the Standard Model and reasons to search for physics beyond the SM, CP symmetry, the concept of effective field theories, the Hilbert series and other useful tools from invariant theory, flavour invariants and topological field configurations in QFT, in particular instantons. These are concepts that will be used throughout this thesis. In particular, the material introduced in Secs. 2.1 and 2.2 covers material relevant for the whole thesis. Secs. 2.3 and 2.5.1 serve as an introduction to Part I of the thesis and Secs. 2.4, 2.5.2 and 2.6 introduce concepts used in Part II of this thesis.

In Chap. 3, based on Ref. [4] we study the νSM, the SM extended with three generations of sterile neutrinos. In an attempt at categorising the sources of CP violation in the νSM, we construct the algebraic ring of flavour invariants built from the flavourful couplings of the theory. We find that there are 459 invariants, out of which 251 are CP-odd and 208 are CP-even that can generate all invariants in the theory as polynomials of them. Using these invariants, we study the seesaw limit of the theory, where the heavy Majorana mass of the sterile neutrinos decouple. Furthermore, in the spirit of the Jarlskog invariant, we formulate the conditions for CP conservation in the theory. We also find some non-trivial cancellations in the plethystic logarithm, a tool from invariant theory that is used to count the number of invariants in the theory and the polynomial relations among them. For two generations of neutrinos, determining the roots of the CP-odd invariants is feasible in a given parameterisation. This allowed us to identify a set of pseudoreal couplings, which have irremovable phases but are still CP-even. This can be easily verified with the flavour invariants.

In Chap. 4, we extend the findings of the νSM in Chap. 3 to the effective operators of the theory studying the sources of CP violation through flavour invariants. We find, that in the absence of sterile neutrinos, the dimension-5 Weinberg operator of the SMEFT only gives rise to flavour invariants at dimension 6 and in order to find flavour-invariant sources of CP violation, one has to consider flavour invariants of dimension 8. For sterile Dirac neutrinos, the flavour structure of the νSMEFT is the same as the one of the quark sector of the SMEFT. Then, more phases of the leptonic operators in the SMEFT become physical, because of the presence of the Yukawa coupling to the right-handed neutrinos. This is also true for the νSMEFT with Majorana sterile neutrinos. Due to the new source of lepton number violation, the phases in the SMEFT Weinberg operator can already appear at dimension 5 as flavour invariants, while the phases of all other additional νSMEFT operators also appear at the leading order in the power counting in a flavour-invariant way.

In Chap. 5, we conclude Part I by summarising our findings and giving an outlook on future research directions.

In Chap. 6, based on Ref. [1] we characterise the shift symmetry of an axionlike particle in the leading order of the effective theory. To this end, we reformulate well-known matrix relations into flavour-invariant quantities. Unlike the matrix relations, they only explicitly depend on couplings of the EFT and the SM Yukawa couplings, are flavour basis-independent and allow to implement the power counting of the shift symmetry-breaking and -conserving part of the theory in a straightforward way. We compute the renormalisation group (RG) equations of the invariants, which form a closed set of differential equations. Furthermore, we perform a matching to UV model to illustrate some features of the invariants. Using the invariants, we can show that shift symmetry in the EFT has a close connection to CP: conservation of CP *almost* implies conservation of the shift symmetry. We also construct the invariants in an EFT with a non-linearly realised electroweak (EW) symmetry and below the EW scale. The construction below the EW scale allows us to apply our invariants to computations of atomic EDMs, where we can derive sum rules on the contribution of the axionlike particle to the EDM based on the invariants. We derive further sum rules with the invariants by considering the contribution of the ALP EFT to the RG running of the SMEFT.

In Chap. 7, based on Ref. [2] we study the implications of the shift symmetry of the ALP on the higher order effective interactions. To this end, we compute the Hilbert series of the ALP EFT with and without a shift symmetry for the ALP and above and below the EW scale. We find a relation between the Hilbert series of the EFT with and without a shift symmetry, that allows us to show that there exist no further equation of motion redundancies like those at dimension 5 exacerbating the implementation of the power counting of the sectors of the ALP EFT with and without a shift symmetry. Using, the Hilbert series, we perform an explicit counting of the operators based on their transformation under CP and divided into operators, which break and conserve baryon and lepton number. Based on these numbers, we build an operator basis for the ALP EFT with and without a shift symmetry for the ALP and above and below the EW scale. We construct a complete set of flavour invariants capturing the leading sources of CP violation in the theory and derive the matrix relations beyond dimension 5, that impose the shift symmetry in the ALP EFT. As an application of our operator basis, we derive positivity bounds for the dimension-8 Wilson coefficients in the ALP EFT above the EW scale.

In Chap. 8, based on Ref. [3] we study how the axion solution to strong CP problem can be spoiled by new sources of CP violation in the UV. For ordinary QCD these effects are suppressed by the scale separation of the QCD scale and the scale of BSM CP violation. This changes in the presence of small instantons, which become important if QCD is modified in a way where the strong coupling increases again in the UV. We construct a set of CP-odd SMEFT flavour invariants featuring the QCD vacuum angle θ better suited for computations in instanton backgrounds. Parameterising the sources of CP violation with the SMEFT, we can show that the axion potential computed from the path integral in the instanton background is proportional to the newly constructed CP-odd SMEFT flavour invariants when all flavourful couplings are kept generic in the computations. Vice-versa, the invariants can be used to systematise the complicated instanton computations. Utilising the bound on the instanton-induced offset of the axion potential minimum implied by the experimental bound on the neutron electric dipole moment, we analyse the constraints imposed on different small instanton and SMEFT flavour scenarios.

In Chap. 9, we conclude Part II by summarising our findings and giving an outlook on future research directions. There, we also conclude the whole thesis by coming back to the questions asked throughout this introduction.

2 Theoretical Foundations

In this chapter, we will introduce all of the technical concepts and tools, we will use throughout this thesis. In Sec. 2.1 we will review the basics of the SM with a focus on CP violation and will give motivations to look for BSM physics. In Sec. 2.2, we will introduce the idea of effective field theory and the most important EFT concepts used in this thesis. We will also introduce the Standard Model effective field theory there. In Sec. 2.3, we will review the generation of neutrino masses, one of the strong motivations for BSM physics. We will show different ways of generating neutrino masses and give a brief overview over neutrino oscillations, which can be used to probe neutrino masses. In Sec. 2.4, we will give an introduction to axions, which are a solution to the strong CP problem. We review the axion mechanism, present some benchmark models of the QCD axion and introduce the EFT of axions and axionlike particles. In Sec. 2.5, we will formalise the concept of invariants in particle physics and introduce important tools from invariant theory like the Hilbert series, the plethyistic logarithm and conformal representation theory. We will show how these tools can be applied to flavour invariants and invariants under gauge and the Poincaré symmetry, simplifying the task of building an operator basis. Finally, in Sec. 2.6, we will introduce topological field configurations and in particular instantons. The material introduced in Secs. 2.1 and 2.2 covers material relevant for the whole thesis. Secs. 2.3 and 2.5.1 serve as an introduction to Part I of the thesis and Secs. 2.4, 2.5.2 and 2.6 introduce concepts used in Part II of this thesis.

2.1 The Standard Model and Beyond

2.1.1 The Standard Model

The development of the Standard Model of particle physics spans centuries of theoretical and experimental efforts of measuring particle physics phenomena and describing those phenomena in the most minimal way in the framework of quantum field theory (QFT). As such, the SM is a combination of the electroweak theory, which unifies the weak and electromagnetic interactions, and quantum chromodynamics, which describes the physics of the strong interactions. The Lagrangian of these theories, describing particle physics with cross-sections spanning several orders of magnitude can be written down in the following incredibly compact

Fields	$L = (\nu_L, e_L)$	e	$Q = (u_L, d_L)$	u	d	H
$SU(3)_c$	**1**	**1**	**3**	**3**	**3**	**1**
$SU(2)_L$	**2**	**1**	**2**	**1**	**1**	**2**
$U(1)_Y$	$-\frac{1}{2}$	-1	$\frac{1}{6}$	$\frac{2}{3}$	$-\frac{1}{3}$	$\frac{1}{2}$

Table 2.1: The SM particle content and its transformation properties under the SM gauge group $SU(3)_c \times SU(2)_L \times U(1)_Y$ following the conventions of Ref. [26]. For each gauge group there exists a multiplet of gauge bosons transforming in the adjoint representation of the group.

way

$$\begin{aligned}\mathcal{L}_{\mathrm{SM}} =& -\frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{4}W^I_{\mu\nu}W^{I,\mu\nu} - \frac{1}{4}G^A_{\mu\nu}G^{A,\mu\nu} + D_\mu H^\dagger D^\mu H + \mu^2 |H|^2 - \lambda |H|^4 \\ &+ \sum_{\psi=Q,u,d,L,e} \bar{\psi} i \not{D} \psi - \left(\bar{L} Y_e H e + \bar{Q} Y_u \tilde{H} u + \bar{Q} Y_d H d + \text{h.c.} \right) + \theta \frac{g_3^2}{32\pi^2} G^A_{\mu\nu} \tilde{G}^{A,\mu\nu}\end{aligned} \tag{2.1}$$

where $I = 1,2,3$ and $A = 1,\ldots,8$ are indices of the adjoint representation of $SU(2)_L$ and $SU(3)_c$, respectively. With $\tilde{H}$ we denote the combination $\tilde{H}_i = \epsilon_{ij} H^*_j$ and $\tilde{G}^{A,\mu\nu} = 1/2 \epsilon^{\mu\nu\alpha\beta} G^A_{\alpha\beta}$, where the ϵs are the 2-index and 4-index totally anti-symmetric tensors. Furthermore, we have suppressed flavour indices of the fermions which come in 3 generations in the SM, making the Yukawa couplings $Y_{u,d,e}$ 3×3 matrices in flavour space. The covariant derivative for a field in the fundamental representation of the SM gauge group is defined as $D_\mu \phi = \left(\partial_\mu + i g_1 Y_\phi B_\mu + i g_2 \tau^I W^I_\mu + i g_3 T^A G^A_\mu \right) \phi$, where T^A are the $SU(3)$ generators, τ^I are the $SU(2)$ generators and Y_ϕ is the hypercharge of the field ϕ.

After electroweak symmetry breaking (EWSB), where the Higgs acquires a vacuum expectation value (VEV) v, the fermions and electroweak gauge bosons receive a mass through the Yukawa couplings of the Higgs to the fermions and the Higgs kinetic term, respectively. We can perform a singular value decomposition on the fermion mass matrices and absorb the appearing unitary matrices by redefining the fermion fields with unitary matrices. We find that we can write the Yukawa couplings as follows[1]

$$Y_e = \mathrm{diag}(y_e, y_\mu, y_\tau)\,, \quad Y_u = \mathrm{diag}(y_u, y_c, y_t)\,, \quad Y_d = V_{\mathrm{CKM}} \mathrm{diag}(y_d, y_s, y_b) \tag{2.2}$$

where V_{CKM} is the Cabibbo–Kobayashi–Maskawa (CKM) matrix, which in the standard parameterisation looks as follows

$$V_{\mathrm{CKM}} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{pmatrix}. \tag{2.3}$$

[1] We have chosen to work in the so-called up-basis, where the up-type Yukawa coupling is exactly diagonal and the CKM matrix V_{CKM} appears in the down-type Yukawa. By making a further redefinition of the quark fields on can also make the opposite choice, where the down-type Yukawa is exactly diagonal and $V^\dagger_{\mathrm{CKM}}$ appears in front of the diagonal up-type Yukawa.

Here, the s_{ij} and c_{ij} are the sine and cosine of the mixing angle of generation i and j and δ is the CKM phase. The CKM matrix appears due to the misalignment of the left-handed up- and down-type quark fields, appearing together in the left-handed quark doublet Q above the scale of electroweak symmetry breaking. While removing the unitary matrices appearing in the singular value decomposition of the Yukawa couplings, the misalignment of the left-handed quark fields leaves the combination $V_{\text{CKM}} = U_{uL}U_{dL}^{\dagger}$, where U_i are the unitary matrices used in the quark field redefinitions to remove unphysical parameters in the Yukawa couplings.

The presence of the CKM matrix in the SM has important physical implications. As we will see in the next section, the presence of the phase δ in the CKM matrix violates a fundamental symmetry of quantum field theory, CP symmetry.

2.1.2 CP Violation in the Standard Model

Effects of CP violation have first been observed in decays of Kaons [27]. Even though all experimental findings at current accuracy can be explained by the CP violation sourced by the SM [25], its origin is still unclear. Understanding effects of CP violation is extremely important, as it might help us understand some potentially hidden structure in the SM quark Yukawa sector that allows us to give an explanation to the so-called flavour puzzle of the SM. Furthermore, it is a vital ingredient in understanding why there exists more matter than antimatter in our universe and how it has been generated in the early universe [24]. We will discuss these issues in more detail below. In this section, we will first lay the ground for understanding the violation of CP in general QFTs and in particular the SM.

To understand this symmetry better, let us study its effect on the Yukawa sector of the SM. Under CP transformations, fermions and scalars transform as follows [28]

$$\begin{aligned}(\mathcal{CP})\psi(t,\vec{x})(\mathcal{CP})^{\dagger} &= e^{i\xi_{\psi}}\gamma^0 C\bar{\psi}^T(t,-\vec{x}) \\ (\mathcal{CP})\phi(t,\vec{x})(\mathcal{CP})^{\dagger} &= e^{i\xi_{\phi}}\phi^{\dagger}(t,-\vec{x})\end{aligned} \tag{2.4}$$

where C is the antisymmetric charge conjugation matrix. Let us first ignore the choice of re-defining the phase of the fields through a CP transformation. Applying these transformations without the rephasing to the Yukawa sector of the SM yields the following conditions on the Yukawa couplings

$$Y_{u,d,e} = Y_{u,d,e}^{*} \tag{2.5}$$

if CP is to be a good symmetry of the model. This means that the phase in the CKM matrix has to vanish in order for the SM to preserve CP. This is the well-known result that imaginary couplings give rise to CP violation. The rest of the SM Lagrangian can be checked to be CP invariant in the form of Eq. (2.1) up to the last term which we will study below.

If we now also take the rephasing possibility of the CP transformation in Eq. (2.4) into account, we can see that we have to slightly modify the condition in Eq. (2.5). In fact, since the fermions in the SM come in flavour multiplets, we can define a CP transformation up to a unitary matrix in flavour space

$$(\mathcal{CP})\psi_i(t,\vec{x})(\mathcal{CP})^{\dagger} = U_{ij}\gamma^0 C\bar{\psi}_j^T(t,-\vec{x})\,, \tag{2.6}$$

where U is a unitary 3×3 matrix in flavour space.[2] Such a CP transformation is called a generalised CP transformation. They have been formally introduced in Ref. [29] and have first been used in Refs. [30, 31] in left-right symmetric models. The condition of CP conservation is modified to

$$Y_{u,d,e} = U_L^\dagger Y_{u,d,e}^* U_R \,, \tag{2.7}$$

where $U_{L(R)}$ is the unitary 3×3 matrix from transforming the left-handed (right-handed) field in the Yukawa interactions. The modified statement about the conservation of CP is that there must exist a flavour basis where the Yukawa couplings are real for CP to be a symmetry of the Lagrangian.[3] Eq. (2.5) should only be used in the 'mass basis' of the theory, where all allowed flavour transformations have already been used to remove unphysical degrees of freedom from the Lagrangian.

With this more general definition of CP it would be convenient to still have a simple relation for CP violation like Eq. (2.5), that does not depend on generic unitary matrices and is instead a basis-independent measure of perturbative CP violation in the SM. This is achieved by the Jarlskog invariant [34–36][4]

$$J_4 = \mathrm{Im}\,\mathrm{Tr}\left([X_u, X_d]^3\right) = 6(y_t^2 - y_c^2)(y_t^2 - y_u^2)(y_c^2 - y_u^2)(y_b^2 - y_s^2)(y_b^2 - y_d^2)(y_s^2 - y_d^2)\mathcal{J} \,, \tag{2.8}$$

where $X_{u,d} = Y_{u,d} Y_{u,d}^\dagger$ and $\mathcal{J} = s_{12} c_{12} s_{13} c_{13}^2 s_{23} c_{23} \sin\delta$. Incredibly, the Jarlskog invariant captures all possibilities of preserving CP perturbatively in the SM; it is zero when CP is preserved and non-zero when CP is violated. Hence, it acts like an order parameter for perturbative CP violation in the SM. One can easily check that the Jarlskog invariant is not only zero when the CKM phase vanishes but also when there exist texture zeros in the CKM matrix that let $\mathcal{J}$ vanish or when quark masses are degenerate or vanishing. This is due to the fact that texture zeros and vanishing or degenerate quark masses lead to a larger exact symmetry group of the SM w.r.t. the case of generic Yukawa couplings, allowing for additional rephasings that can remove the CKM phase from the Lagrangian.

There is another source of CP violation in the SM Lagrangian that we have neglected so far. The last term in Eq. (2.1), the so-called θ-term, is also CP-violating.[5] This can be easily

[2]This unitary matrix allows for new exact flavour symmetries of the Lagrangian. Indeed, applying CP twice on the Lagrangian gives rise to a transformation in flavour space by the matrix UU^*. The ordinary CP transformation is the one, where $UU^* = \mathbb{1}$. However one can also define an order n CP transformation by demanding that $(UU^*)^n = \mathbb{1}$.

[3]In the presence of discrete symmetries not even that has to hold true. In that case there can exist pseudo-real couplings with complex entries which cannot be removed in any basis, yet they still conserve CP. This is due to the fact that because of the discrete symmetry the Lagrangian parameters are such that they can be turned into their complex conjugate by this discrete transformation. Combining a CP transformation with this discrete transformation leads to CP conservation. For more details see Refs. [4, 32, 33] and App. 3.E.2.

[4]We will derive the form of the invariant more systematically later in Sec. 2.5.1, where we will also discuss the cases where the exact flavour symmetry group of the SM is increased, leading to CP conservation.

[5]Note, that in principle there could also be a corresponding term for the other SM gauge fields. There is no corresponding term for the hypercharge gauge boson B, because there is no non-trivial way of wrapping a $U(1)$ gauge boson configuration on the symmetry group of the 4-dimensional space-time boundary (in mathematical language: the corresponding homotopy group is trivial) [37]. The $SU(2)_L$ θ-term can be rotated away in the SM due to the chirality and anomaly structure of the SM. Indeed, $SU(2)_L$ only has a mixed anomaly with $B+L$ transformations. Since, all SM interactions are $B+L$-conserving, the electroweak θ-angle can be rotated

seen by appreciating that the kinetic term of the gluons preserves CP. The only difference to the θ-term is the 4-dimensional Levi-Civita symbol $\epsilon^{\alpha\beta\gamma\delta}$, which behaves as a tensor density under space-time transformations. Tensor densities transform with the determinant of the transformation matrix [41]. While C leaves the Levi-Civita tensor unchanged, the parity transformation represented by $P = \mathrm{diag}(1,-1,-1,-1)$ yields a non-trivial transformation

$$\epsilon^{\alpha\beta\gamma\delta} \xrightarrow{CP} \det P \epsilon^{\alpha\beta\gamma\delta} = -\epsilon^{\alpha\beta\gamma\delta} . \tag{2.9}$$

However, this term does not appear in perturbation theory as it can be written as a total derivative which vanishes at the boundary unless some non-trivial boundary conditions are imposed. We will explore topological configurations with such non-trivial boundary conditions in Sec. 2.6 and their appearance in models of new physics in Chap. 8. The θ-term is at the centre of one of the yet unsolved problems of the SM. Even though it is allowed by the SM gauge symmetries and even anthropic arguments only give weak bounds on its coefficient [42], CP violation is measured to be absent in the strong interactions to large accuracy. Indeed, the best measurement of CP violation in the strong interaction, the electric dipole moment (EDM) of the neutron implies the incredible bound of [43][6]

$$\bar{\theta} \lesssim 10^{-10} , \tag{2.10}$$

where we have defined the physical θ parameter $\bar{\theta} = \theta + \arg\det(Y_u Y_d)$, which is invariant under rephasings of the SM quark fields. On the other hand, the θ parameter is expected to be of $\mathcal{O}(1)$ from a naturalness point of view. This discrepancy is known as the strong CP problem. Its most famous solution is the axion which we will explore in Sec. 2.4 and aspects of it in Part II of this thesis.

2.1.3 Peeking at What Lies Beyond

Let us now look at the problems of the SM, that could give a hint in our search towards a theory of everything. The problems of the SM can be loosely put into two categories: serious problems of the SM, where the theory does not reproduce phenomena observed in Nature and aesthetic problems of the theory, where the SM works perfectly fine as a phenomenological description of Nature, but we are unsatisfied with some of its features. Let us start with the first category.

One problem of the SM is that it does not explain the neutrino masses in Nature observed in neutrino oscillations. Indeed, due to the gauge structure of the SM, no masses are generated

away and has no physical effect in the SM [38–40]. This can change in UV completions of the SM, where $B+L$ is violated.

[6]Note, that this value is due to an analysis where the θ-term is taken as the single source for the neutron EDM. While this is a good approximation in the SM due to the flavour suppression of CP violation in the SM, this must not hold true for BSM physics. There, CP violation could be less (or even not at all) flavour suppressed and has only evaded detection so far due to its decoupling behaviour going as E/Λ, where E is the energy scale of the experiment and Λ is the scale associated with the new physics. Effects of heavy new physics on the neutron EDM through other sources than the θ term have been studied in effective theories in Refs. [5, 44–48].

for the left-handed neutrinos ν_L of the SM. Only at the non-renormalisable level of the SM Lagrangian neutrino masses can be generated, as we will explore in Sec. 2.3.

Another issue is that the SM does not give an explanation for the baryon asymmetry of the universe, based on the observation that there exists much more matter than anti-matter in the universe. This can be understood with the mechanism of baryogenesis, explaining an excess generation of baryons in the early universe, if the Zakharov conditions [24] hold true. These require sizeable CP violation (beyond that provided by the SM, which is too small for a successful baryogenesis), baryon number violation and a state of non-equilibrium between the baryon number-violating reactions, such that more baryons than anti-baryons are generated.

The SM also does not have a dark matter candidate accounting for the 27% [49] of the total energy density in the universe that exists in the form of matter that can only have very feeble interactions with electromagnetic radiation. Effects of the dark matter can be observed in rotation curves of galaxies [50] or through gravitational lensing effects of light around galaxies [51].

Another mystery of Nature is what the fundamental quantum theory of gravity looks like and if it can be unified with the other forces of Nature. We know that our current geometrical understanding of gravity thanks to Einstein is just an effective theory that should break down at the Planck scale, where quantum effects of gravity become strong [52]. However, it is highly questionable if such scales can ever be directly probed experimentally. Therefore, trying to understand the phenomena of gravity to high precision in an effective approach might help us learn about its UV quantum theory.

Furthermore, even though the SM itself is by now well-tested, some details of it are not fully understood yet. For instance, in the strong sector the details of QCD confinement are yet to be fully appreciated and in the electroweak sector, for example, it has not been verified yet if the realisation of electroweak symmetry breaking is indeed linear as in the SM or if it should be of non-linear nature, which can be probed by the tri-linear coupling of the Higgs boson [53].

Let us now come to the aesthetic problems of the SM, which can all be summarised by our dissatisfaction of not understanding the value of parameters of the SM. For instance, it is a mystery, why the Yukawa couplings are hierarchical and why they come in the existing hierarchy. This is also referred to as the flavour puzzle. Even though it seems strange that such a hierarchy should exist, it does not diminish the power of the SM at describing phenomena, but it leaves us unsatisfied because we would like to have an explanation for those hierarchies, ideally in terms of a dynamic theory that reduces the amount of parameters necessary to describe Nature.

The same is true for the strong CP problem. We are unsatisfied with the smallness of the θ parameter. What is even more puzzling in the case of the strong CP problem is that the symmetry which could in principle forbid the θ-term is broken in the SM. Hence, the vacuum angle θ could take on any large value that would not change Nature drastically.

There are another two hierarchy problems related to the quantum corrections of mass parameters in QFT. The first one is the smallness of the cosmological constant compared to the Planck mass and the other problem is the smallness of the Higgs mass compared to the Planck mass.

We will only comment on the second one here, because it is more straightforward to pin down in QFT. The smallness of the Higgs mass compared to the Planck mass is called a hierarchy problem because the Higgs receives quantum corrections to its mass, which unlike the mass of gauge bosons or fermions are not protected by any symmetry in the SM. Therefore, these corrections can naively be as large as the Planck mass or should at least be as large as the mass of the new physics resonances we expect to resolve the problems of the SM. For the Higgs mass to be at its physical value, some tuning is required between the bare mass in the Lagrangian and the quantum corrections which can be much larger than the tree-level contribution should new physics be sufficiently heavy.

However, in theories where the Higgs mass is not predicted by the theory and is just an input parameter, as is the case of the SM as a phenomenological description of the Higgs sector, the quantum corrections just amount to redefining this arbitrary input parameter. In theories where the Higgs mass is predicted and correlated with other quantities in the theory, the tuning problem is a real problem in keeping the prediction of the Higgs mass close to its measured value while still keeping consistency with all other predictions of the theory with measurements. Therefore, a more useful question might be to understand the fundamental theory behind the phenomenological description of the Higgs sector in the SM, that provides explanations for the details of breaking of EW symmetry, the stability of the Higgs potential and in particular, the origin of the Higgs mass.

Indeed, the SM does not have any fundamental problems as a QFT, like Landau poles or unitarity problems [54], and could therefore work up to extremely high scales to make accurate predictions for phenomena observed in particle physics, excluding the serious problems discussed above.

Many theories have been proposed to address the problems listed in this section, however in recent years no direct signal of new particles have been found in experiments. There are two ways to add new physics while evading detection with current experiments. New physics could either be light and extremely weakly coupled, such that even though we could directly produce the new particles, the production cross-section is extremely small. BSM physics could also be heavy, such that we can not produce it directly and we can only study the effects of the heavy new physics by performing experiments to high precision in order to find the new physics as small deviations from the theoretical prediction of the SM. In this thesis we approach both of these scenarios by accepting the extreme success of the SM and taking its effective nature seriously. We will study both decoupling heavy new particles in the effective theory of the SM, but will also study two cases, where light particles exist that have to be included in the effective description of physics at low energies. In the next section, we will introduce the concept of effective field theories in more detail.

2.2 Effective Field Theory

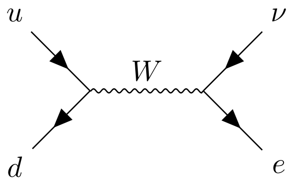
In our endeavour of finding the fundamental theory of Nature it can be useful to take a step back and take a precise look at our current understanding of phenomena. In fact, we do this all the time in our every day life as a physicist. When trying to understand the macroscopic properties of an electric circuit we would never start to think about the details of "how every single electron moves along the circuit", which become irrelevant at macroscopic distances, but instead use quantities like its resistance and Ohm's Law. There are many more examples of this among all of Physics, like the multipole expansion in Electrodynamics [55], where a complicated charge configuration can be approximated at long distances, or the Ginzburg–Landau theory [56] in condensed matter theory, which is a phenomenological description of type-I superconductors, modelling them without the knowledge of the underlying Cooper pairs, which are the degrees of freedom of the more fundamental Bardeen–Cooper–Schrieffer description of superconductors. All of these examples have one common feature: there is a separation of two characteristic scales, which we will call Λ_L and $\Lambda_H \gg \Lambda_L$ in the following. This scale separation allows to study the physics at the low scale Λ_L with the relevant degrees of freedom decoupled from the high scale Λ_H, as we will see in a second. We will use this basic concept in the context of QFT, to describe similar problems as we have just discussed in the realm of particle physics, where a separation of two or more characteristic scales exists.

There are two ways to use EFTs, the bottom-up and the top-down approach. In the top-down approach the full theory is known and an EFT can be helpful to reorganise the theory in terms of the relevant degrees of freedom – this is for example the case in chiral perturbation theory (χPT) of QCD –, to improve the convergence of the perturbative expansion – this is often used in flavour physics to resum large logarithms –, or to study certain kinematical setups of particle interactions of interest at colliders – this is for instance done in soft collinear effective theory. In the bottom-up approach the full fundamental theory at a high energy scale is not known. Instead, the effective theory is constructed by considering the known particle spectrum and all symmetries of the theory at low energies. Then, the effective theory can be used to investigate phenomena of Nature precisely in order to find small deviations from what we think is the current best theory of Nature to get some hints about a more fundamental theory instead of looking for new physics directly.

Let us discuss a more specific example that is of high historical importance showing that EFTs have been used well before their technical development – Fermi's 4-fermion interactions. For a long time physicists were puzzled by the nuclear β decay, which lets a neutron decay to a proton, an electron and an anti-neutrino – an at the time unknown particle. In the advent of quantum field theory, it was Fermi's genius to postulate this new particle and describe the β decay as an interaction between the four mentioned particles [57, 58]. In our modern understanding, the theory can be understood as the transition of a down-quark to an up-quark in the neutron with the simultaneous emission of the electron and neutrino. This interaction can be described by the Lagrangian

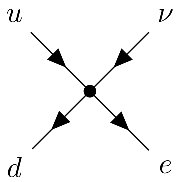
$$\mathcal{L}_{\text{Fermi}} = G_F \, \bar{d}_L \gamma_\mu u_L \, \bar{\nu}_L \gamma^\mu e_L + \text{h.c.}\,, \tag{2.11}$$

which is local, i.e. all fields interact at a single point space-time point. We want to stress here that this interaction of four fermions only contains left-handed fermions. With the development of the SM, we have understood the interactions to come from the charged current interactions of the W boson with the left-handed quark and lepton doublets in Eq. (2.1). In the SM, the process can be described by the following transition amplitude



$$= \left(-i\frac{g}{\sqrt{2}}\bar{d}\gamma^{\mu}P_L u\right)\frac{-ig_{\mu\nu}}{p^2 - m_W^2}\left(-i\frac{g}{\sqrt{2}}\bar{\nu}\gamma^{\nu}P_L e\right), \tag{2.12}$$

where d, u, ν, e are external spinors of the fermions, $P_L = \frac{1-\gamma^5}{2}$ with γ^5 the fifth gamma matrix and we have used the propagator of the W boson in Feynman gauge. Expanding the propagator of the W boson in the small quantity $p^2/m_W^2 \ll 1$ allows us to understand the Lagrangian in Eq. (2.11) as the effective interaction of the charged current interactions of the SM mediated by the W boson. Note, that the effective 4-fermion interaction is a local contact interaction at a single space-time point. Hence, at low energies we can understand the effects of the heavy resonance as a space-time local interaction by shrinking down the propagator of the heavy resonance, as the propagating heavy new particle can no longer be resolved at low energies. Indeed, at low energies from the point of view of the Fermi Lagrangian in Eq. (2.11), we see



$$= iG_F\left(\bar{d}\gamma^{\mu}P_L u\right)\left(\bar{\nu}\gamma^{\nu}P_L e\right). \tag{2.13}$$

Should on the other hand another effective operator made from all the low-energy degrees of freedom below the electroweak scale have been measured in experiment, we could have learned about its origin through the Lorentz and gauge structure of this effective interaction. A charged heavy scalar, for example, would have generated the effective operator $\bar{d}_L u_R\, \bar{\nu}_L e_R$+h.c. at low energies instead.

At this point we should question ourselves where the effective theory is valid. The series expansion of the propagator obviously only makes sense when the energy scale of the process p^2 is much small than the mass of the W boson. The characteristic scale of the theory set by $G_F \sim \frac{1}{\Lambda^2}$ yields an energy scale of about $\Lambda \sim 300$ GeV for the effective theory. Furthermore, taking the EFT in Eq. (2.11) at face value, the theory will run into unitarity issues (i.e. probabilities will be larger than 1, making the theory nonsensical) at a scale $4\pi G_F^{-\frac{1}{2}}$. This is an important point because $p^2 \sim m_W^2$ is where the heavy particle goes on resonance, whereas G_F is the characteristic scale of the 4-fermion interaction. Comparing the couplings in the effective and the full theory, we find that

$$\frac{G_F}{\sqrt{2}} = \frac{g^2}{8m_W^2} = \frac{1}{2v^2}. \tag{2.14}$$

Therefore, parametrically $m_W \sim gG_F^{-\frac{1}{2}}$, which for a perturbative coupling g is much lower than the characteristic scale of the theory. In summary, even though the theory only breaks down at a scale $4\pi G_F^{-\frac{1}{2}}$, the theory is UV-completed at a scale $m_W < G_F^{-\frac{1}{2}}$, where the heavy particle goes on resonance, and should only be trusted to the scale of the lightest new resonance.

All of these aspects have been formalised in the last few decades. The use of EFTs to describe the effects of heavy new particles at energies well below their mass is based on the decoupling theorem [59]. However, there are exceptions to this theorem, in particular in the case of chiral theories including couplings to the Higgs. One famous example is a fourth sequential generations of chiral fermions, which receive their mass from the Higgs mechanism. Because their mass generation is connected to the electroweak sector, they can never be decoupled from the theory. In the meantime this scenario has been ruled out experimentally [60, 61]. A catalogue of such non-decoupling particles can be found in Ref. [62].

Excluding such cases and working in a bottom-up approach the most general EFT can be built by considering the known particle spectrum at low energies and building all operators allowed by the Poincaré, gauge symmetries and optionally other global symmetries that one believes should be considered.[7] Then, the EFT Lagrangian can be written down generically in the following way

$$\mathcal{L}_{\text{EFT}} = \mathcal{L}^{(\leq 4)} + \sum_{d>4,i} C_i^{(d)}(\Lambda_H, \mu) \frac{\mathcal{O}_i^{(d)}(\Lambda_L, \mu)}{\Lambda_H^{d-4}}, \tag{2.15}$$

where $\mathcal{L}^{(\leq 4)}$ collects all the relevant and marginal couplings among the light degrees of freedom, d is the mass dimension of the respective operator and Λ_L and Λ_H are the characteristic low- and high-energy scales. μ is the so-called matching or renormalisation scale, where the heavy particles are integrated out from the theory and is often chosen to be the heavy scale $\mu \sim \Lambda_H$. Finally, $C_i^{(d)}$ are the so-called Wilson coefficients of the effective operators, modelling the correct non-analytic behaviour of the full theory at low energies in terms of only the light degrees of freedom that enter the effective operators $\mathcal{O}_i^{(d)}$.

We naturally expect the Wilson coefficients to be of $\mathcal{O}(1)$ at the matching scale and because only the light degrees of freedom appear in observables at low scales, we have $\langle \mathcal{O}^{(d)} \rangle \sim \Lambda_L^{d-4}$ for Green's functions with an insertion of an effective operator of mass dimension d. Since the effective operators $\mathcal{O}^{(d)}$ of mass dimensions d are suppressed by $\Lambda_H^{-(d-4)}$, we can organise our computations in the EFT by the parameter

$$\lambda = \frac{\Lambda_L}{\Lambda_H} \ll 1, \tag{2.16}$$

which is called the *power counting* of the EFT. Even though this observation is quite simple, it is an important and powerful aspect of effective theories.

[7] For example, the SMEFT is often used under the assumption of exact lepton and baryon number conservation (which are accidental symmetries of the SM Lagrangian), even though there exist operators at dimension 5 and 6 in the SMEFT breaking those symmetries explicitly. These symmetries are, however, only violated at very high scales above $\sim 10^{14}$ GeV in theories like grand unified theories [63], making them good symmetries in practice.

2.2.1 Operator Bases

While constructing the higher-dimensional operators there are some redundancies that one should keep in mind in order not to work with an over-complete set of operators.

Integration by parts redundancies The first redundancy is rather straightforward and concerns the use of integration by parts (IBP) in effective actions. As the action is defined as the space-time integration over the Lagrangian density, one can always redefine the Lagrangian in a way where the action is left invariant together with possible integral transformations. We will discuss this for IBP transformations following an example presented in Ref. [64]. We define a generic effective theory with an operator basis containing two Poincaré and gauge-invariant operators $\mathcal{O}_{1,2}$ satisfying the following relation

$$\mathcal{O}_1 = \mathcal{O}_2 + \partial_\mu \mathcal{O}_3^\mu \,. \tag{2.17}$$

In the action, we can then write with generic Wilson coefficients

$$\begin{aligned} S \supset \int_V d^4x\ C_1\mathcal{O}_1 + C_2\mathcal{O}_2 = \int_V d^4x\ C_1\left(\mathcal{O}_2 + \partial_\mu \mathcal{O}_3^\mu\right) + C_2\mathcal{O}_2 = \int_V d^4x\ \left(C_1 + C_2\right)\mathcal{O}_2 \\ + \oint_{\partial V} d^3x\ C_1 n_\mu \mathcal{O}_3^\mu = \int_V d^4x\ C_2'\mathcal{O}_2 \,. \end{aligned} \tag{2.18}$$

Here, n_μ is a normal vector of the boundary ∂V of the integration volume V. We have used Gauss's law and the fact that all fields do not have support on the integration boundary at infinity. In the last step we have simply redefined the arbitrary Wilson coefficient of the operator.

It is evident that only one of the operators has to be kept in a non-redundant operator basis. We say that the two operators are equivalent by IBP if they have a redundancy as in Eq. (2.17). The physical interpretation of this is more straightforward by studying the amplitudes with an insertion of those operators. The redundancy in Eq. (2.17) leads to a relation between the amplitudes of the operators of the following form [64]

$$F_1\left(\{p_i\}\right) \sim F_2\left(\{p_i\}\right) + \left(\sum_i p_{i,\mu}\right) F_3^\mu\left(\{p_i\}\right) \,, \tag{2.19}$$

where the F_i are polynomials of the momenta p_i. Hence, IBP redundancies correspond to momentum conservation $\sum_i p_i^\mu = 0$ at the level of the amplitudes.

Equation of motion redundancies The other more involved redundancy are equation of motion (EOM) redundancies that can be removed when S-matrix elements instead of Green's functions are computed. This is due to the fact that imposing the kinematic on-shell relation in S-matrix elements reduces the amount of independent Lorentz invariants that can appear, allowing the same physics to be captured by a smaller amount of operators. One can prove that operators including the classical EOM of the theory can be removed via field redefinitions [65],[8] which we will show here for a single scalar field along the lines of Ref. [67]. With the path integral

$$Z[J] = \int D\phi\, e^{i\int \mathcal{L}[\phi]+J\phi} \tag{2.20}$$

of a QFT in mind, the fields can be understood as mere integration variables and redefinitions of them are allowed. One particularly useful class of field redefinitions that can be used to remove the EOM redundancy we just mentioned are those proportional to the EOM of the field obtained by varying the action $\frac{\delta S}{\delta \phi}$. It is quite straightforward to see that operators proportional to the EOM

$$\theta[\phi] = F[\phi]\frac{\delta S}{\delta \phi}\,, \tag{2.21}$$

cannot contribute to S-matrix elements and can instead be traded for operators with less derivatives, reducing the size of the overall operator basis significantly. To see this we simply employ the following Ward identity for Green's functions that will later be reduced to S-matrix elements

$$\langle 0|T\{\phi(x_1)\ldots\phi(x_n)\theta[\phi]\}|0\rangle = i\sum_i \delta^{(4)}(x-x_i)\langle 0|T\{\phi(x_1)\ldots\cancel{\phi(x_i)}\ldots\phi(x_n)F[\phi(x_i)]\}|0\rangle\,. \tag{2.22}$$

To obtain the S-matrix element, the LSZ reduction formula has to be applied putting all external particles on their mass shell. In order to do this, the Green's function has to be multiplied by inverse propagators $p_i^2 - m^2$ for every external particle cancelling the poles in the propagators of the external particles. However, each term in the sum on the right-hand side of Eq. (2.22) misses one of these poles due to the contact term in the form of the δ-function. Hence, S-matrix elements with insertions of operators proportional to the classical EOM of the theory vanish and these operators can be excluded from the operator basis. The proof for fermions and vector fields goes along the same lines and we will not show it here.

Note, that this does not hold true when calculating (off-shell) Green's functions as a vital step in the proof was putting the fields on shell and amputating the external propagators. In that case, EOM operators have to be kept and this enlarged basis is usually called an off-shell or Green's basis with respect to the physical or on-shell basis mentioned before.

Besides the redundancies mentioned so far, there exist also redundancies due to relations in the different group algebras under which the fields transform. For instance, there exist Fierz identities among 4-fermion operators due to relations in the Clifford algebra, which relate certain operator structure reducing the amount of operators that have to be considered in a complete operator basis. Similar relations also exist for the gauge groups.

There is one last redundancy connected to the choice of operator basis, which is relevant to radiative loop computations with insertions of effective operators. In dimensional regular-

[8] Removing redundant operators will generally lead to infinite (in the sense of having a $1/\epsilon$ pole in dimensional regularisation) anomalous dimensions of fields or Green's functions with remaining infinities (because the corresponding operator structures acting as counter terms have been removed via field redefinitions) [66]. Once the S-matrix is computed, these infinities will drop out as expected since the S-matrix is invariant under field redefinitions. For an example of such an infinite field redefinition that yields infinite Green's functions, see the end of Chapter 6 of Ref. [67]. We have encountered a similar example in Ref. [5].

isation [18], where divergent integrals are regulated by going to $d = 4 - 2\epsilon$ dimensions, some identities used to simplify Dirac and Lorentz structures appearing in computations change. For instance, in 4 dimensions $\mathrm{Tr}\,(\gamma^\mu\gamma^\nu) = 4\eta^{\mu\nu}$, while in d dimensions $\mathrm{Tr}\,(\gamma^\mu\gamma^\nu) = (4-2\epsilon)\eta^{\mu\nu}$. Whenever these additional ϵ pieces hit $1/\epsilon$ poles in loop computations before ϵ is taken to zero, the finite terms are changed. Evanescent operators exactly capture the additional pieces proportional to ϵ coming from identities of space-time dimension-dependent objects in the operator basis. They live in d dimensions and disappear when ϵ is taken to zero.

2.2.2 Matching and Running

In this section, we will introduce important technical aspects of EFTs that will be used throughout this thesis: matching and running. In short, matching is the process of linking the effective theory to specific UV models by expressing the Wilson coefficient in terms of fundamental UV parameters and we denote as running the handling of the behaviour of Wilson coefficients under the change of energy scales, which can be used to resum large logarithms that can appear in computations.

Matching We have already seen one example of matching in the Fermi theory above, but will state the procedure in more generality here. The goal of matching is to determine the Wilson coefficients of the effective theory, such that the effective theory models the behaviour of the full theory at low energies without including the heavy degrees of freedom. There are different approaches to achieve this. The simplest approach, that traditionally has been most popular, is the one of matching renormalised on-shell matrix elements. For the matching, as many independent processes are chosen as there are independent Wilson coefficients in the EFT at a given precision. Then, the renormalised on-shell amplitudes of the full theory and the effective theory are equated at the matching scale μ_M

$$i\mathcal{M}^{\mathrm{EFT}}_{\mathrm{ren}}(\mu_M) = i\mathcal{M}^{\mathrm{full}}_{\mathrm{ren}}(\mu_M)\,, \tag{2.23}$$

where the amplitude in the full theory is expanded in the low energy scale(s) divided by the heavy mass scale of the particle that is integrated out and in the EFT the amplitude is computed only with the operators up to the mass dimension needed to reach the accuracy of interest. To leading order, only the tree-level amplitudes of the EFT and full theory are considered and the Wilson coefficients are determined in terms of the full theory couplings. If a higher accuracy is desired, the amplitudes for the given processes used for the matching have to be computed to a higher loop order, after which the Wilson coefficients are again determined as a function of the full theory parameters. To get accurate EFT results, the scale dependence of the Wilson coefficients should be considered, as will be discussed below.

Another possibility is functional matching, in which the heavy particles are directly integrated out in the path integral. This is why matching is also often referred to as integrating out the heavy particle from the theory. Arguments based on the path integral approach are often used to perform the tree-level matching between the full theory and the EFT. Let us define a simple UV theory with action $S_{\mathrm{UV}}(\phi, \Phi)$, where ϕ is a light field and Φ is a heavy field, that can be integrated out from the theory as follows

$$e^{iS_{\rm EFT}(\phi)} = \int \mathcal{D}\Phi \; e^{iS_{\rm UV}(\phi,\Phi)} . \tag{2.24}$$

To obtain the leading tree-level matching we can expand the UV action around its classical configuration, that dominates the path integral. To this end, we compute the classical equation of motion of the heavy field $\frac{\delta S_{\rm UV}(\phi,\Phi)}{\delta\Phi} = 0$ and formally solve it for the heavy field $\Phi = \Phi_c(\phi)$. Plugging the classical solution for the heavy field back into the action yields the tree-level-matched effective action of the theory

$$S_{\rm EFT}^{\rm tree}(\phi) = S_{\rm UV}(\phi, \Phi = \Phi_c(\phi)) , \tag{2.25}$$

corresponding to the saddle point approximation of the path integral. To obtain the loop-level matching, we have to also consider the quantum fluctuations η around the classical solution Φ_c of the heavy fields, i.e. we split $\Phi = \Phi_c + \eta$. Then, we find [68]

$$e^{iS_{\rm EFT}(\phi)} = e^{iS_{\rm UV}(\phi,\Phi=\Phi_c)} \int \mathcal{D}\eta \; \exp\left(\frac{i}{2}\frac{\delta^2 S}{\delta\Phi^2}|_{\Phi=\Phi_c}\,\eta^2 + \mathcal{O}\left(\eta^3\right)\right) . \tag{2.26}$$

which is a Gaussian integral in the quantum fluctuations that can be solved systematically [69, 70]. Recently, some computer programmes have been developed, both based on diagrammatic matching [71] and functional matching [72–74], that automate the matching procedure.

Running Usually, observables are measured at low scales, while the EFT operators are generated by integrating out some heavy particles at comparably high scales. Therefore, it is important to correctly keep track of the scale dependence of the Wilson coefficients to make accurate predictions for observables in terms of the EFT parameters. To keep track of the scale dependence of the Wilson coefficients, one defines the so-called renormalisation group equation (RGE) of the Wilson coefficients C_i

$$\mu\frac{dC_i}{d\mu} = \gamma_{ij} C_j , \tag{2.27}$$

where γ_{ij} is the anomalous dimension of the Wilson coefficients. We want to emphasise here, that in the RGE of Wilson coefficient C_i other Wilson coefficients C_j can appear, which is usually denoted as operator mixing. This has the important consequence that even if some Wilson coefficient vanishes at the matching scale, it can be generated by the appearance of another Wilson coefficient in the RGEs, which is non-zero at the matching scale. The RGEs of an EFT can be computed by removing the UV divergences appearing in loop computations by a renormalisation procedure of the couplings and fields of the theory. In particular, we define[9]

$$\Phi^{(0)} = \sqrt{Z_\Phi}\Phi, \quad C^{(0)} = Z_C \mu^{n\epsilon} C \tag{2.28}$$

[9]Here and in the following, C and Z_C can be matrices in the space of EFT operators.

where the superscript (0) denotes bare objects, while the objects without a superscript are the renormalised couplings and fields. Furthermore, $\epsilon = (4-d)/2$ is the regulator of dimensional regularisation, n is an integer that depends on the mass dimension of the operator to be renormalised and the Z_i are the renormalisation constants of the couplings and fields. By demanding that the bare coupling does not depend on the scale of renormalisation, we find

$$\mu\frac{dC^{(0)}}{d\mu} = \mu\frac{d(\mu^{n\epsilon}Z_C C)}{d\mu} = \left(n\epsilon + C^{-1}\mu\frac{dC}{d\mu} + (Z_C)^{-1}\mu\frac{dZ_C}{d\mu}\right)\mu^{n\epsilon}Z_C C \overset{!}{=} 0\,. \tag{2.29}$$

After simplifying this expression, we find

$$\mu\frac{dC}{d\mu} = -n\epsilon C - (Z_C)^{-1}\frac{dZ_C}{dC}\mu\frac{dC}{d\mu}C \tag{2.30}$$

which can be used to compute the RGE of the EFT, by renormalising the theory at a given loop order to obtain the renormalisation constant Z_C and subsequently evaluating Eq. (2.30) with the explicit expressions. The RGEs of the EFT Wilson coefficients are indispensable at making accurate predictions within the EFT and are, for instance, commonly used to resum terms with large logarithms of the type $\left(\frac{g^2}{16\pi^2}\log\frac{\Lambda_H^2}{\Lambda_L^2}\right)^p$ [67, 75].

Note, that in EFT computations the RGEs are often used to estimate the EFT contribution to processes. Here, the 'leading log' approximation is used, where Eq. (2.27) is solved by evolving the Wilson coefficient with the presciption

$$C_i(\Lambda_L) \approx C_i(\Lambda_H) + \gamma_{ij}C_j\log\left(\frac{\Lambda_H}{\Lambda_L}\right) \tag{2.31}$$

from a high scale Λ_H (where the EFT is matched to another EFT or a UV-complete theory) to the low scale Λ_L, where observables are computed. Then for a sufficient separation of scales, the logarithm in the expression gives the dominant piece, whereas the finite threshold correction $C_i(\Lambda_H)$ at the matching scale is often ignored. However, depending on the operator, the logarithm does not always have to become extremely large. For instance, taking the scale of new physics Λ_H to be 10 TeV and roughly take 100 GeV for the heavy particles in the SM, we get

$$\log\frac{\Lambda^2}{m_{\text{EW}}^2} \approx \log\left(\frac{10\text{ TeV}}{100\text{ GeV}}\right)^2 = 2\log(100) \approx 10\,. \tag{2.32}$$

Therefore, assuming a rational term of $\mathcal{O}(1)$ gives a correction of $\mathcal{O}(10\%)$. Moreover, when an operator does not run under the RG flow at all, the finite threshold contribution can even be the leading piece. We have studied this in Ref. [5] in the context of electric dipole moments at 1-loop in the SMEFT.

A comment about the renormalisability of EFTs is in order. It can be shown that a sufficient but not necessary condition for a theory to be renormalisable is, that it only contains operators of mass dimension 4 and lower. This can be done by counting the so-called superficial degree of divergence [76]. A proof was first sketched by Dyson for quantum electrodynamics [77] and later formalised and generalised to other theories (see for instance Ref. [78]).

From a modern point of view of renormalisability, a theory is renormalisable when enough renormalisation constants in the theory exist to absorb all divergences that appear in perturbative loop computations, even if an infinite number of those constants is needed [79]. In this sense effective theories are also renormalisable. Starting from a 4-dimensional Lagrangian, that we know is renormalisable by considering the superficial degree of divergence, one can start adding effective operators at the next order in the power counting. By inserting a single power of these operators into loop diagrams, one can absorb all UV divergences by absorbing them into the counterterm of these operators. An apparent problem appears when two or more of these operators are inserted. Then, UV divergences are generated that can only be absorbed by adding a counterterm from an operator that appears at the mass dimension that is obtained by summing the mass dimension of the inserted operators. Therefore, more and more operators have to be added to absorb all divergences and the theory seems to become non-predictive.

To resolve this apparent problem, one has to keep the power counting of EFTs in mind. On top of the small couplings of the renormalisable Lagrangian that are used as an expansion parameter in perturbation theory of QFTs, the EFT is also an expansion in its power counting parameter. As mentioned before, in an EFT computation the working precision in the power counting is always specified and any effects that are more suppressed in the power counting of the EFT can be ignored. Therefore, multiple insertions of EFT operators that seem to be problematic can actually be ignored at a fixed working precision and no counterterm operator of higher mass dimension has to be added. Thus, the renormalisability of EFTs is saved.

2.2.3 The Standard Model Effective Field Theory

As was made clear throughout this chapter, we know that new physics beyond the SM must exist. However, no clear direct signal has been observed in recent years in experiments guiding us the way to the right UV completion, that resolves (some of) the issues of the SM. In this case, the effective nature of the SM should be taken seriously, and the higher order interactions among the SM degrees of freedom should be taken into account, which effectively capture the effect of some decoupled heavy new physics. In this setup, one can look for deviations of measurements from the SM prediction in a fairly model-independent way. There is another useful aspect of the SMEFT: it can be used as a book keeping tool for new physics models. Should at some point an experimental anomaly with substantial significance be found, the SMEFT can be used to easily identify which UV completions can lead to such an anomaly thanks to dictionaries [80, 81] translating between the SMEFT operators, in terms of which the anomaly can be easily computed at the leading EFT order, and specific (simplified) UV completions.

In the following, we will assume that the electroweak symmetry is linearly realised, i.e. we will work with the Higgs doublet of the SM. Some UV models require a non-linear realisation of the EW symmetry group, which does not allow for a matching of these models to the SMEFT [82, 83]. Instead, an EFT based on the gauge group $SU(3)_c \times U(1)_{em}$ should be built, where the physical Higgs h is treated as a singlet under the gauge group independently of the Goldstone modes of the EW gauge bosons, which are packaged into a matrix of Goldstone bosons $U = \exp\left(i\pi^i\tau^i/v\right)$ [84]. This EFT is usually referred to as the chiral SM effective Lagrangian or the Higgs effective field theory (HEFT).

Assuming that EW symmetry is indeed realised linearly, the SMEFT Lagrangian can be obtained by constructing all operators made from the SM fields allowed by Poincaré and SM gauge symmetries and removing all IBP and EOM redundancies. The SMEFT Lagrangian can be expanded as follows

$$\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \frac{\mathcal{L}^{(5)}}{\Lambda} + \frac{\mathcal{L}^{(6)}}{\Lambda^2} + \dots, \tag{2.33}$$

where the power counting of the theory is simply E/Λ with E the characteristic energy of the process under consideration and Λ the characteristic scale, where new physics is expected to appear. Due to recent experimental non-observations of new particles beyond the SM we expect $\Lambda \gg E$, making the SMEFT expansion well-behaved.

At mass dimension 5 only one operator is allowed by Poincaré invariance and the SM gauge symmetries. This is the so-called Weinberg operator [63]

$$\mathcal{O}_5 = \left(\bar{L}^c\tilde{H}^*\right)\left(\tilde{H}^\dagger L\right), \tag{2.34}$$

providing a Majorana mass for the left-handed SM neutrinos after EWSB. This operator breaks lepton number and is therefore often excluded from SMEFT analyses.

At mass dimension 6 all hell breaks loose and there exist 84 operators for one generation of fermions and 3045 operators for the three generations present in the SM [85]. A first basis at dimension 6 has been constructed a few decades ago [86], but has only been made completely non-redundant in the last decade [87]. With the development of tools like the Hilbert series and methods based on Young tableaux, operator bases up to dimension 12 have been derived [88–93].

Furthermore, the 1-loop RGEs for the dimension-6 Wilson coefficients in the Warsaw basis have been computed in Refs. [94–97], which are invaluable in making accurate SMEFT predictions at low energy scales (compared to where new physics is expected), where all experiments conducted by humanity run.

Before we continue with discussing CP violation in the SMEFT, we first want to discuss how to use EFTs in practice. In this thesis we will use EFTs in the bottom-up approach, where the following procedure should be adhered to. At first, the desired accuracy of the computation is fixed, both in the loop expansion and the EFT power counting. Fixing the accuracy in the power counting fixes the mass dimension up to which operators should be kept in the EFT after which a complete and non-redundant operator basis can be built.

For a desired precision of $\lambda^2 = v^2/\Lambda^2 \sim 0.1\%$, Λ can be at most up to a few TeV, in which case logarithms generated by the scale dependence of Wilson coefficients are relatively small $\log\left(\Lambda/m_W\right) \sim 3$ [68]. To achieve per mille level precision in the loop counting, it is sufficient to compute up to the 1-loop order. Hence, for an operator which is typically generated at tree-level [98], processes should be computed at 1-loop accuracy, whereas for operators which are generated at higher loops tree-level accuracy is sufficient.

To reduce the complexity of the EFT, which in light of the 3045 Wilson coefficients of the

SMEFT at dimension 6 is often desirable, some minimal assumptions can be made about the UV physics. Usually, lepton and baryon number are assumed to be conserved, motivated by the non-observation of such processes to high accuracy. Since most of the complexity in the SMEFT comes from the flavourful Wilson coefficients, many assumptions concern the flavour sector of the UV scenario. Some common assumptions are flavour-universal couplings – where all flavourful couplings are proportional to the identity–, minimal flavour violation (MFV) [99–101] – where the SM Yukawa couplings are taken to be the only flavourful parameters in the UV[10] – and an anarchic flavour scenario – where all entries of the flavourful Wilson coefficient matrix are simply of $\mathcal{O}(1)$. Another possibility is to focus on some sector of the EFT, like the Higgs sector, for which the assumption of strong coupling in the UV, for instance, allows for the organisation of the operators into the SILH basis [102].

Then, sufficiently many observables are computed in the EFT to constrain all the free parameters in the EFT at the given accuracy and after potentially applying some assumptions about the UV. One can either perform a global fit in the bottom-up approach to study small deviations from the SM predictions or set one-operator bounds by only turning on one operator at a time to get a feeling for the limit on the scale of new physics. In the top-down approach one can integrate out specific models and study their behaviour at low energies.

A particularly interesting class of UV completions are those which come with additional sources of CP violation w.r.t. the SM. CP is violated by the weak interactions in the SM, hence it should not come as a surprise if there exists more CP violation in BSM physics. Indeed, there are many good motivations to look for CP violation beyond the SM. On the one hand, CP violation from BSM physics is necessary to understand the baryon asymmetry of the Universe through baryogenesis. On the other hand, we have never been closer to identifying if there is CP violation in the neutrino sector, which also necessarily hints at new physics, because interactions giving rise to neutrino masses do not exist within the SM (c.f. Sec. 2.3). Furthermore, the strong CP problem is another problem connected to this symmetry, that calls for further study.

Another important aspect is that due to the flavour suppression of CP violation in the SM captured by the Jarlskog invariant, most CP-violating observables have a tiny SM background. This makes them exceptional probes of new physics, as any signal in the big window to the SM background would be a clear sign of new physics. Some key CP-violating observables are EDMs of leptons and composite objects like nucleons and atoms, CP violation in meson systems, and asymmetries of differential cross sections with respect to CP-odd triple products measured at particle colliders. Hence, it is an important task to study CP-violating new physics in a systematic way by employing EFT tools, which we will discuss now in the context of the SMEFT.

CP violation in the SMEFT The non-renormalisable interactions of the SM degrees of freedom give rise to new sources of CP violation, that effectively capture the sources of CP violation of decoupling UV theories with a linearly realised EW symmetry. At dimension

[10]MFV can be understood as having flavour-universal couplings in the UV, which after matching at the UV are evolved to low energies with the RGEs of the EFT. Since the only non-trivial flavour tensors in the RGEs will be the Yukawa couplings, the Wilson coefficients at a lower energy scale will follow MFV.

5, the Weinberg operator contains 6 CP-odd couplings that can be identified by applying the CP transformation rules introduced in Eq. (2.4). At dimension 6 there already exist 1149 CP-odd couplings for the three generations of fermions in the SM [97]. Out of these, six correspond to bosonic operators and the remaining sources of CP violation come from operators with fermions, subject to the ambiguity of a choice of flavour basis resolved by the Jarlskog invariant in the SM. Since all observables should not depend on any choice of mathematical basis, they should be expressible in terms of flavour invariant quantities which are independent of the choice of a *flavour* basis, capturing all source of CP violation in the SMEFT at a given order in the EFT expansion. For instance, many observables in particle physics are defined through scattering processes, which are characterised by (differential) scattering cross sections and quantities derived thereof, which depend on the modulus square of the matrix element. When a computation is performed in the SMEFT, the leading order SMEFT correction will usually appear at dimension 6 and the amplitude including the leading order correction to the SM can be written as $\mathcal{M} = \mathcal{M}_4 + \mathcal{M}_6$, where $\mathcal{M}_4$ is the SM piece and $\mathcal{M}_6$ is the SMEFT piece. Then, the square of the matrix element reads

$$|\mathcal{M}|^2 = |\mathcal{M}_4 + \mathcal{M}_6|^2 = |\mathcal{M}_4|^2 + 2\mathrm{Re}\left(\mathcal{M}_4 \mathcal{M}_6^*\right) + \mathcal{O}\left(\frac{1}{\Lambda^4}\right). \tag{2.35}$$

Here, the dominating piece of the SMEFT corrections is usually the interference piece between the SM and the SMEFT, if the process allows for an interference between the SM and SMEFT contributions and if the dimension-8 contributions are more suppressed than the interference term, which is usually the case. The invariants also give hope for an organising principle as to which sources of CP violation are the most important, due to the flavour suppression introduced by the SM Yukawa couplings appearing in the flavour invariants.

Therefore, it will be interesting to construct objects which are linear in the CP-odd dimension-6 Wilson coefficients and do not depend on the choice of flavour basis. Such a categorisation has recently been performed in Refs. [103, 104], which we will briefly review here. The goal is to construct a minimal set of flavour invariants capturing the sources of CP violation in the SMEFT at $\mathcal{O}(1/\Lambda^2)$. Inspired by the Jarlskog invariant, the SMEFT invariants should also capture all sources of CP violation in the case of an increased exact flavour group of the SM due to degenerate masses or texture zeros in the CKM matrix.

To show that a constructed set of flavour invariants captures the necessary and sufficient condition for CP conservation in the presence of a given effective operator, we will use the transfer matrix introduced in Ref. [103] making use of the linearity of the flavour invariants in the Wilson coefficient. The transfer matrix is defined as the linear map between the entries of the Wilson coefficients arranged into a vector and the invariants

$$\mathcal{I}_a\left(C\right) = \mathcal{T}_{ai}\,\vec{C}_i\,, \tag{2.36}$$

where $\mathcal{T}$ is the transfer matrix and $\vec{C}_i = (\mathrm{Re}\,C_{11}, \mathrm{Re}\,C_{12}\,\ldots, \mathrm{Im}\,C_{11}, \mathrm{Im}\,C_{12}\,\ldots)$ is the vector of the entries of the Wilson coefficient, which we have shown here for an operator with a fermion bilinear. The transfer matrix has a block-diagonal form $\mathcal{T} = \left(\mathcal{T}^R\ \mathcal{T}^I\right)$, where for the majority of this thesis we will ignore the block $\mathcal{T}^R$ because it corresponds to the CP-even

EFT flavour invariants. Due to the linearity of the transfer matrix in the Wilson coefficient, it can only depend on the SM Yukawa couplings. By checking if the block $\mathcal{T}^I$ of the transfer matrix has full rank, i.e. the rank is equal to the number of phases in the Wilson coefficients that cannot be removed by field redefinitions, for random[11] numerical values of the Yukawa couplings, we can check if the set indeed captures all necessary and sufficient condition for CP conservation. For more details see Ref. [103], where also the maximal ranks for all CP-odd operators in the Warsaw basis of the dimension-6 SMEFT are given.

We will discuss three examples to illustrate the main results of Ref. [103]. For the first example, we will discuss the Yukawa-like operator $\mathcal{O}_{uH} = |H|^2\bar{Q}\tilde{H}u$, whose Wilson coefficient has nine complex parameters. All of the nine CP-violating parameters are physical and cannot be removed with flavour transformation from the Lagrangian. Hence, we can find nine flavour invariants that capture those sources of CP violation

$$\begin{aligned} &L_{0000}\left(C_{uH}Y_u^\dagger\right), L_{1000}\left(C_{uH}Y_u^\dagger\right), L_{0100}\left(C_{uH}Y_u^\dagger\right)\\ &L_{1100}\left(C_{uH}Y_u^\dagger\right), L_{0110}\left(C_{uH}Y_u^\dagger\right), L_{2200}\left(C_{uH}Y_u^\dagger\right)\\ &L_{0220}\left(C_{uH}Y_u^\dagger\right), L_{1220}\left(C_{uH}Y_u^\dagger\right), L_{0122}\left(C_{uH}Y_u^\dagger\right). \end{aligned} \tag{2.37}$$

Here, $L(C)$ is defined as $L_{abcd}(C) = \operatorname{Im}\operatorname{Tr}\left(X_u^a X_d^b X_u^c X_d^d C\right)$. Together with the Jarlskog invariant J_4 defined above, the roots of these invariant capture the necessary and sufficient conditions for CP conservation in the SM extended with the operator $\mathcal{O}_{uH}$. We want to note here, the flavour suppression of some of these invariants due to the smallness of the SM Yukawa couplings. Comparing them to the Jarlskog invariant shows that new CP violation could well be less suppressed than in the SM, given that the EFT scale suppression together with the flavour suppression in the SMEFT invariants is not as severe as that of the Jarlskog invariant in the SM. This is also true for non-zero J_4, as is realised in Nature, where the simple presence of a new *CP-even* flavour structure in the UV, is enough to have CP violation less suppressed than in the SM [104]. We want to highlight another aspect here, which the SMEFT invariants make transparent: just like in the SM, CP violation is a collective effect in the SMEFT, which requires the conspiracy of several Lagrangian parameters in order for the symmetry to be violated.

As the second example, we consider the hermitian operator $\mathcal{O}_{Hq}^{(1)}$, whose Wilson coefficient due to the hermitian property only has three off-diagonal CP-odd parameters. Again, all sources of CP violation are physical and can be written in a flavour-invariant way

$$L_{1100}\left(C_{Hq}^{(1)}\right), L_{2200}\left(C_{Hq}^{(1)}\right), L_{1122}\left(C_{Hq}^{(1)}\right). \tag{2.38}$$

Note, that the first invariant in this set contains terms which have the least amount of SM Yukawa couplings among the invariants in this set and hence is the least suppressed by small quantities. Therefore, in a computation, we would expect this invariant to appear earliest in computations, due to its small amount of SM coupling insertions, and also be the most important numerically, since it is the least suppressed. However, one has to keep in mind,

[11] The values have to be random in a way where they do not give rise to exact flavour symmetries of the renormalisable SM Lagrangian.

that these SMEFT invariants could still appear in observables divided by other SM flavour invariants, such that the hierarchy of which is the most important invariant could be changed. In Chap. 8, we will show a scenario, where all the SMEFT flavour invariants indeed appear in computations without further suppressions by other SM invariants.

Finally, we want to discuss the lepton dipole operator $\mathcal{O}_{eB}$, whose Wilson coefficient also allows for nine phases. If one tries to write down all possible CP-odd flavour invariants linear in the Wilson coefficient, one will find the following set of invariants

$$\mathrm{Im}\,\mathrm{Tr}\left(C_{eB}Y_e^\dagger\right), \quad \mathrm{Im}\,\mathrm{Tr}\left(X_e C_{eB}Y_e^\dagger\right), \quad \mathrm{Im}\,\mathrm{Tr}\left(X_e^2 C_{eB}Y_e^\dagger\right). \tag{2.39}$$

Due to the structure of the lepton Yukawa sector, no other independent CP-odd flavour invariants can be written down at the leading order in the dimension-6 SMEFT Wilson coefficient. Hence, at the leading order not all phases in this leptonic Wilson coefficient can appear in a flavour-invariant way in observables. We will call phases which can appear in flavour invariants linear in the Wilson coefficients *primary phases* and all phases which can only appear in a flavour-invariant way at higher orders in the EFT *secondary phases*. Due to this non-interference effect in the leptonic sector of the SMEFT, only 705 out of the 1149 sources of CP violation can appear in a flavour-invariant way at the leading order in the EFT [103]. This has recently been confirmed by a Hilbert series counting of CP-violating couplings in the SMEFT [105].

This changes in the presence of neutrino masses. Depending on the Dirac or Majorana nature of this mass term, the non-interference effect at the leading order in the EFT could be lifted, as we will explore in Chap. 4.

2.3 Neutrino Masses

Due to $SU(2)_L$ gauge invariance, the left-handed neutrinos ν_L appearing in the lepton doublet L do not receive a mass term in the renormalisable SM. This follows directly from the fact that all fermion mass terms in the SM are chiral and the left-handed neutrino does not have a right-chiral partner as all other SM fermions do. Indeed, expanding the Higgs in the lepton Yukawa coupling in Eq. (2.1) around its VEV, we find (only keeping terms proportional to the VEV)

$$\mathcal{L}_{\mathrm{SM}} \supset -\bar{L}Y_e H e + \mathrm{h.c.} = -\bar{e}\, Y_e \frac{v}{\sqrt{2}} P_R\, e + \mathrm{h.c.}\,, \tag{2.40}$$

but no corresponding term including the neutrino ν_L. This is in contradiction with measurements of neutrino oscillations [106, 107], which are only compatible with massive neutrinos.

There are two fundamentally different ways to realise a mass for the neutrinos. The first one can be understood by going to low energies, where the left-handed neutrino is a singlet of the SM gauge group. Them, one can write down a mass term even without adding any new matter to the theory

$$\mathcal{L}_\nu = \bar{\nu}_L i\partial\!\!\!/ \nu_L - \left(\frac{1}{2}\bar{\nu}_L m_\nu \nu_L^c + \mathrm{h.c.}\right). \tag{2.41}$$

If one tries to find the UV roots of this operator in terms of the building blocks which linearly realise the electroweak symmetry, the search will only be successful at the non-renormalisable level with the Weinberg operator $\mathcal{O}_5$ introduced in Eq. (2.34). This term gives rise to a Majorana mass term for the left-handed neutrino

$$\mathcal{L}\nu \supset \bar{\nu}_L i\partial\!\!\!/\nu_L + (C_5\mathcal{O}_5 + \text{h.c.}) = \bar{\nu}_L i\partial\!\!\!/\nu_L - \left(\bar{\nu}_L^c \frac{v^2 C_5}{2\Lambda}\nu_L + \text{h.c.}\right), \tag{2.42}$$

where we have again only kept terms proportional to the Higgs VEV. The most simple UV completions of this term are the seesaw models, where a heavy singlet right-handed neutrino [108–113], a heavy $SU(2)$ triplet right-handed neutrino [114–117] or an $SU(2)$ triplet scalar [118] is added to the theory, generating the Weinberg operator at tree level when integrated out. There are also models generating the neutrino masses at loop level, going under the name of scotogenic models [115, 119–121]. See also Refs. [122–124] for systematic studies of the radiative generation of the Weinberg operator at higher loop orders and Ref. [125] for a review of radiative neutrino mass models.

The other possibility is to add a light right-chiral partner of the left-handed neutrino to the theory. This light sterile neutrino allows to write down the following Lagrangian

$$\mathcal{L}_{\nu\text{SM}} = \mathcal{L}_{\text{SM}} + \bar{N}i\partial\!\!\!/N - \left(\bar{L}Y_N\tilde{H}N + \frac{1}{2}\bar{N}^c M_N N + \text{h.c.}\right), \tag{2.43}$$

which goes under the name of νSM [126–130] in the literature. Just like in the SM, the additional couplings that are added to the theory by extending it with right-handed neutrinos can introduce new sources of CP violation in the theory. This calls for a basis-invariant study of CP violation as we have discussed for the SM in Sec. 2.1.2. CP violation in the neutrino sector is particularly interesting, as current experimental measurements are not yet conclusive about the size or even existence of CP violation in the neutrino sector. We will study this in more detail now.

After applying a single value decomposition on the matrices appearing in the Lagrangian a mixing matrix, like the CKM matrix in the quark sector appears. The exact form of the matrix depends strongly on the mechanism responsible for neutrino mass generation and in particular the Majorana or Dirac character of neutrinos. We will discuss this in detail in App. 3.A. Here, we will restrict ourselves to the case, where there exist 3 light Majorana neutrinos at low energies. This is for instance the case when the mass of the SM neutrinos is generated through the Weinberg operator by some UV completions like the seesaw mechanism. Then, the mixing matrix, the Pontecorvo–Maki–Nakagawa–Sakata (PMNS) matrix, can be written as follows in the standard parameterisation [25]

$$U_{\text{PMNS}} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{pmatrix} \cdot \begin{pmatrix} e^{i\eta_1} & 0 & 0 \\ 0 & e^{i\eta_2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{2.44}$$

which is a CKM-like matrix with 3 mixing angles and a phase, which we will refer to as the

Dirac phase, multiplied by another matrix with two more phases. The two phases $\eta_{1,2}$ are only present due to the Majorana character of the neutrinos which does not allow to rotate them away by rephasings of the fields. If instead there exist light right-handed neutrinos and lepton number is conserved, i.e. a Majorana mass term is forbidden, the Lagrangian of the theory is that in Eq. (2.43) with M_N set to zero. Then, the lepton Yukawa sector has the same structure as that of the quark sector and the PMNS matrix has the same form as the CKM matrix.

The PMNS matrix has important physical consequences. If the PMNS matrix is non-trivial, it will lead to oscillations of neutrinos between different flavour states. We will briefly review this effect here following the review in Ref. [25]. Let us define a weak neutrino eigenstate ν_α related to the mass eigenstates ν_i by the PMNS matrix

$$|\nu_\alpha\rangle = U^*_{\alpha i}|\nu_i\rangle \,. \tag{2.45}$$

After the state is produced by the weak interaction, we can evolve the state in time in its mass basis. After some time t, where the neutrino has travelled a distance $L = t$,[12] we can describe the state as

$$|\nu_\alpha(t)\rangle = U^*_{\alpha i}|\nu_i(t)\rangle \,, \tag{2.46}$$

where we assume that the wave function of the neutrino is simply that of a plane wave $|\nu_i(t)\rangle = e^{-iE_i t}|\nu_i(0)\rangle$. Starting with a neutrino in the weak eigenstate $|\nu_\alpha\rangle$, the probability of a neutrino being in the flavour state $|\nu_\beta\rangle$ after some time t has passed is

$$P_{\alpha\beta} = |\langle\nu_\beta|\nu_\alpha(t)\rangle|^2 = |U^*_{\alpha i}U_{\beta j}\langle\nu_j|\nu_i(t)\rangle|^2 \,. \tag{2.47}$$

Taking the neutrinos to be relativistic and approximately of the same energy, i.e. $|\mathbf{p}_i| \simeq |\mathbf{p}_j| \equiv p \approx E$, we can expand the energies of the neutrinos appearing in the time evolution as follows

$$E_i = \sqrt{\mathbf{p}_i^2 + m_i^2} \approx p + \frac{m_i^2}{2E} \,. \tag{2.48}$$

Then, assuming proper normalisation of the neutrino mass states we find for the oscillation probability

$$P_{\alpha\beta} = \delta_{\alpha\beta} - 4 \sum_{i,j=1,i<j}^{3} \mathrm{Re}\left(U_{\alpha i}U^*_{\beta i}U^*_{\alpha j}U_{\beta j}\right)\sin^2\left(X_{ij}\right) + 2 \sum_{i,j=1,i<j}^{3} \mathrm{Im}\left(U_{\alpha i}U^*_{\beta i}U^*_{\alpha j}U_{\beta j}\right)\sin\left(2X_{ij}\right) \,, \tag{2.49}$$

where $X_{ij} = \frac{(m_i^2 - m_j^2)L}{4E}$. Measurements of these oscillations allow to constrain the difference in the square of the masses, as well as the mixing angles and Dirac phase of the PMNS matrix. Measurements can either be made by using neutrinos generated in the sun, which requires the prediction of the neutrino flux of the sun, or neutrinos from nuclear reactors, which allow for an easier estimate of the flux due to the better controlled environment, and subsequently detecting them with large detectors sensitive to the elusive particles. Note here,

[12] Due to their small mass we can take neutrinos to be relativistic.

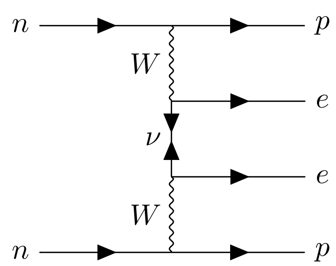


Figure 2.1: Feynman diagram of a neutrinoless double beta decay, which is only possible due to the Majorana nature of the intermediate neutrino.

that the measurements only allow to measure the difference in the square of the masses of the neutrinos. Current measurements are compatible with a hierarchical neutrino mass spectrum: $m_2^2 - m_1^2 \ll m_3^2 - m_2^2$ [25], which allow for a normal ordering ($m_1 < m_2 \ll m_3$) or an inverted ordering ($m_3 \ll m_1 < m_2$). The mass itself can only be measured by other means. The KATRIN experiment, for instance, looks for tiny deviations in the tail of the energy spectrum of beta decays of tritium (which has a particularly low-energetic beta decay) to determine the effective mass $m_\nu^2 = \sum_i |U_{ei}|^2 m_i^2$. The current best limit by KATRIN is $m_\nu < 0.8$ eV [131].

The Dirac phase can be determined by measuring the probability of a neutrino to oscillate from one flavour to another and taking the difference to the same oscillations with anti-neutrinos [132]. Because the probability of the anti-neutrino oscillations is the same as those for neutrinos computed in Eq. (2.49) after replacing $U \to U^*$, we find

$$P_{\alpha\beta} - P_{\bar{\alpha}\bar{\beta}} = 4 \sum_{i,j=1,i<j}^{3} \mathrm{Im}\left(U_{\alpha i} U_{\beta i}^* U_{\alpha j}^* U_{\beta j}\right) \sin\left(2X_{ij}\right) . \tag{2.50}$$

Note, that this expression is proportional to the reduced equivalent of the Jarlskog invariant in the neutrino sector, which is defined in the same way as the Jarlskog invariant of the quark sector in Eq. (2.8). This calls for an analysis of these measurements in terms of invariants. To this end, we construct a generating set of invariants for the νSM in Chap. 3. Note also, that the Majorana phases drop out of the expression in Eq. (2.50), because the same Majorana phase multiplies a whole column of the CKM-like matrix in Eq. (2.44). The measurement of the Dirac phase is extremely difficult. Even though good progress is made by oscillation experiments, the phase is still not known to high accuracy. Curiously, current measurements in normal ordering of neutrino masses is still compatible with the CP-conserving point $\delta = \pi$ [133]. Measuring a non-zero value for one of the phases in the neutrino sector could help understanding the matter-antimatter asymmetry via leptogenesis [134].

The Majorana nature of neutrinos can be determined in neutrinoless double beta decays [135, 136]. As can be seen in Fig. 2.1, this process is only possible when the neutrino has a Majorana mass compatible with the lepton number-violating nature of the decay $nn \to ppee$. To date, no experimental evidence of these decays have been found and the current best limit for the half-life of such a process has the impressive value of $T_\beta^{0\nu} > 2.3 \cdot 10^{26}$ years [137].

2.4 Axions and Axionlike Particles

2.4.1 The Axion Solution to the Strong CP Problem

We have already introduced the strong CP problem in Sec. 2.1.2. In summary, it is the question why the θ-parameter, the coefficient of the term $G_{\mu\nu}\tilde{G}^{\mu\nu}$, is so small. By now, the probably most famous solution to the strong CP problem is the axion solution. The idea is to dynamically relax the parameter to zero, by introducing a new particle whose potential is such that it is minimised for $\bar{\theta} = 0$. To achieve this, a new $U(1)$ symmetry – often referred to as Peccei-Quinn (PQ) symmetry – is postulated in the UV, which is spontaneously broken by the VEV of a scalar field [138, 139]. This gives rise to a Goldstone boson [140, 141], the axion, which due to its Goldstone nature does not have a potential and is therefore a priori massless. In order to generate a potential for the axion field a, which relaxes $\bar{\theta}$ to zero, the PQ symmetry needs to have a mixed anomaly with QCD, yielding the interaction $aG\tilde{G}$ between gluons and the axion, adding to the QCD θ-term as follows

$$\mathcal{L} \supset \left(\frac{a}{f_a} + \bar{\theta}\right) G\tilde{G}\,. \tag{2.51}$$

It is now convenient to make use of the shift symmetry of the axion to absorb $\bar{\theta}$ into the axion field. When QCD confines, the term $a/f_a G\tilde{G}$ will give rise to a periodic potential for the axion breaking the shift symmetry of the axion to a discrete symmetry $U(1) \to \mathbb{Z}_N$(with N the anomaly factor of the mixed QCD–PQ anomaly) [142] , minimised at zero. Historically, instantons – semi-classical topological tunnelling solutions of QCD to be studied in more detail in Sec. 2.6 below – were thought to have a major role in the confinement dynamics of QCD. Therefore, some early attempts of computing the QCD axion potential made use of large-sized, i.e. low-energy, QCD instanton configurations, leading to the well-known cosine potential [20, 143, 144]

$$V(a) \propto e^{-\frac{8\pi^2}{g_3^2}} \left(1 - \cos\frac{a}{f_a}\right)\,, \tag{2.52}$$

where f_a is the axion decay constant. This potential is evidently minimised at $\langle a/f_a \rangle, = \bar{\theta} = 0$ and thus, the strong CP problem is solved. We will however see in Sec. 2.6 that instantons are no longer reliable, when the QCD coupling becomes non-perturbative (as can be seen from the exponential in Eq. (2.52)) and χPT should be used instead to compute the potential of the axion [145]. In that case, the potential was found to be [145, 146]

$$V(a) = -m_\pi^2 f_\pi^2 \sqrt{1 - \frac{4m_u m_d}{(m_u + m_d)^2}\sin^2\left(\frac{a}{2f_a}\right)}\,, \tag{2.53}$$

which is aligned with the instanton cosine potential but has a significantly different form. As for the instanton-induced potential it can also be easily checked that the potential in Eq. (2.53) is minimised at $\langle a/f_a \rangle, = \bar{\theta} = 0$, hence solving the strong CP problem. Expanding the potential in Eq. (2.53) to quadratic order gives the well-known mass relation [140]

$$m_a f_a = \sqrt{\frac{4 m_u m_d}{(m_u + m_d)^2}} m_\pi f_\pi \,, \tag{2.54}$$

making the QCD axion extremely light compared with to particles appearing in the SM. Including next-to-leading order (NLO) corrections to the potential, the QCD axion has a mass of $m_a \approx 5.7\ \mu\text{eV} \frac{10^{12}\text{GeV}}{f_a}$ [145]. Due to the lightness of the axion and its generic (as we will see below) weak coupling to the SM particles, axions are also a prime candidate for dark matter [144, 147–150].

It has been proven [151] that CP is preserved in parity-conserving vector-like theories such as QCD with a θ-term and extended by an axion. This is of course no longer true in the SM, which is a chiral theory and has additional sources of CP violation through the CKM matrix as we saw earlier. These sources can feed into the axion potential and off-set its minimum. These contributions are called misaligned contributions as they are not aligned with the potential generated by QCD and will give corrections to the minimum. The aligned corrections are phase-aligned with the QCD axion potential and only change the mass of the axion with respect to the QCD axion. We will study these effects later in Chap. 8, where we study small size, i.e. high-energy, instanton contributions to the axion potential with new sources of CP violation in the UV parameterised by SMEFT operators.

Another important aspect, that relates to the Goldstone nature of the axion as well, is the fact that the $U(1)$ symmetry is by construction anomalous and hence, not a good symmetry of the Lagrangian (see for instance Ref. [142] for a recent review). Furthermore, in the most common constructions the PQ symmetry is a global symmetry of the Lagrangian. It has been shown [152–163], that quantum gravity does not allow for exact global symmetries and will introduce irreducible corrections to the axion Lagrangian of the form

$$V(\phi) \supset \frac{\phi^n}{M_{\text{Pl}}^{n-4}} \,, \tag{2.55}$$

where $\phi \sim f_a e^{i\frac{a}{f_a}}$ is the scalar that Higgses the PQ symmetry. At the current experimental accuracy for the bound on the θ parameter, these interactions break the axion solution to the strong CP problem unless $n \gtrsim 14$ [164]. This usually goes under the name of the *axion quality problem* in the literature, questioning the existence of a PQ symmetry that has a sufficiently high quality in suppressing PQ-breaking interactions enough in order for the strong CP problem to still be solved at the accuracy dictated by experiment. Common solution to this problem are introducing accidental discrete symmetries – such that the terms allowed to appear in Eq. (2.55) are harmless –, considering a composite axion – where instead of a PQ scalar, the axion arises from a composite operator, which has a high quality if its scaling dimension is sufficiently large –, or introducing the axion through a higher-dimensional gauge field – where the shift symmetry is then protected by the gauge symmetry respected by quantum gravity [142].

To close this section, we also want to briefly present alternative solutions to the strong CP problem. The simplest solution is the massless up-quark solution, where the vanishing of a quark mass introduces a chiral symmetry allowing to rotate the θ-term away and thus rendering it unphysical. This solution has been ruled out by lattice simulations of quark masses, proving that all quarks are massive [25, 165]. Another popular class of solutions is based on spontaneously breaking an explicit CP or P symmetry in the UV. The first model based on this construction is the Nelson–Barr model [166, 167].

2.4.2 Benchmark Models of the QCD Axion

Soon after the idea of the axion emerged, efforts were made to come up with UV realisations of the mechanism. There are three noteworthy models we will present in the following of which the last two are often used as benchmark models for the QCD axion.

The Weinberg–Wilczek model The Weinberg–Wilczek (WW) model [140, 141] is probably the simplest UV realisation of an axion model based on the SM gauge group. The model is extending the SM with another Higgs doublet to a Two-Higgs-Doublet model (2HDM)

$$\mathcal{L} \supset \bar{Q} g_1 H_1 u + \bar{Q} g_2 H_2 d + \text{h.c.} + V(H_1, H_2)\,, \tag{2.56}$$

which allows for a PQ symmetry of the form

$$u \to e^{i\alpha} u, \quad d \to e^{i\beta} d, \quad H_1 \to e^{-i\alpha} H_1, \quad H_2 \to e^{-i\beta} H_2\,. \tag{2.57}$$

After both of the Higgs doublets receive a VEV v_1 and v_2, respectively, there exists one linear combination of scalars which is CP-odd and, as the Goldstone boson of the spontaneously broken PQ symmetry, does not receive a potential

$$a = -\sin\beta\ \text{Im}H_1^0 + \cos\beta\ \text{Im}H_2^0\,. \tag{2.58}$$

Here, H_i^0 is the neutral component of the Higgs bosons and $\tan\beta = v_1/v_2$. In the model the axion decay constant can be computed to be [140, 141]

$$f_a = \frac{v}{6} \sin 2\beta\,, \tag{2.59}$$

where $v = \sqrt{v_1^2 + v_2^2}$ is the EW scale. Due to the closeness of the axion decay constant in this model to the EW scale $v \simeq 246$ GeV the model (and simple variations of it) have quickly been ruled out by experiment [150].

The Kim–Shifman–Vainshtein–Zakharov model In the Kim–Shifman–Vainshtein–Zakharov (KSVZ) model [168, 169], the SM is extended by a single heavy vector-like quark $\mathcal{Q} = \mathcal{Q}_L \oplus \mathcal{Q}_R$, transforming as $(\mathbf{3}, \mathbf{1})_0$ under the SM gauge group and a singlet complex scalar Φ, which has the role of decoupling the PQ breaking scale from the EW scale. This set-up allows for the following Lagrangian

$$\mathcal{L}_{\text{KSVZ}} = \mathcal{L}_S M + \partial\Phi^\dagger \partial\Phi + \bar{\mathcal{Q}} i \not{D} \mathcal{Q} - \left(y_{\mathcal{Q}} \Phi \bar{\mathcal{Q}}_L \mathcal{Q}_R + \text{h.c.}\right) - V(|\Phi|, |H|)\,, \tag{2.60}$$

where a bare mass term $\bar{\mathcal{Q}}\mathcal{Q}$ has been forbidden by imposing the discrete symmetry $\mathcal{Q}_L \to -\mathcal{Q}_L, \mathcal{Q}_R \to \mathcal{Q}_R, \Phi \to -\Phi$ [168]. This Lagrangian has an accidental PQ symmetry, realised as

$$\mathcal{Q}_L \to e^{i\alpha}\mathcal{Q}_L, \mathcal{Q}_R \to e^{-i\alpha}\mathcal{Q}_R, \Phi \to e^{2i\alpha}\Phi\,. \tag{2.61}$$

The potential of the scalars

$$V(\Phi, H) = -\mu_\Phi^2|\Phi|^2 - \mu_H^2|H|^2 + \lambda_H|H|^4 + \lambda_\Phi|\Phi|^4 + \lambda_{H\Phi}|\Phi|^2|H|^2 \tag{2.62}$$

is such that the PQ symmetry is broken at a scale f by the VEV of Φ. It is convenient to parameterise the scalar in polar coordinates around its VEV

$$\Phi = \frac{1}{\sqrt{2}}\left(f + \rho\right) e^{i\frac{a}{f}}\,, \tag{2.63}$$

where the axion can be identified with the massless angular excitation a, while as usual, the radial excitation ρ receives a large mass and can be integrated out. After spontaneous PQ breaking, the Yukawa coupling of the heavy quarks now has the following dependence on the axion

$$\mathcal{L}_{\text{KSVZ}} \supset -\frac{y_\mathcal{Q} f}{\sqrt{2}}\bar{\mathcal{Q}}_L\mathcal{Q}_R e^{i\frac{a}{f}} + \text{h.c.}\,. \tag{2.64}$$

After performing a chiral transformation $\mathcal{Q}_L \to e^{ia/(2f)}\mathcal{Q}_L, \mathcal{Q}_R \to e^{-ia/(2f)}\mathcal{Q}_R$ on the heavy quark anomalously changing the $G\tilde{G}$-term, the heavy quarks are PQ neutral and can be integrated out from the model. Generated by this chiral transformation, we recognise the familiar axion-gluon interaction term

$$\mathcal{L}_{\text{KSVZ}} \supset \frac{g_3^2}{32\pi^2}\frac{a}{f}G\tilde{G}\,, \tag{2.65}$$

which after confinement of QCD gives a potential to the axion that solves the strong CP problem.

The Dine–Fischler–Srednicki–Zhitnitsky model The Dine–Fischler–Srednicki–Zhitnitsky (DFSZ) model [170, 171] is a slight modification of the WW model, where the axion decay constant is decoupled from the EW scale by adding an additional singlet complex scalar Φ to the model which transforms as a singlet under the SM gauge group and a PQ charge of +1. The scalar potential can then be written as

$$V(H_1, H_2, \Phi) = V(|H_1|, |H_2|, |\Phi|, |H_1^\dagger H_2|) + \lambda H_1^\dagger H_2 \Phi^{\dagger 2} + \text{h.c.} \tag{2.66}$$

Depending on the type of 2HDM, there are several ways to couple the two Higgs doublets to the SM fermions. Choosing for definiteness a type-I 2HDM, we have the following Yukawa couplings

$$\mathcal{L}_{\text{DFSZ}} \supset -\bar{Q}Y_u H_1 u - \bar{Q}Y_d H_2 d - \bar{L}Y_e H_2 e + \text{h.c.}\,. \tag{2.67}$$

The potential of the scalars is now chosen such that all scalars receive a VEV. We can parameterise the scalars in polar coordinates around their VEVs

$$H_1 \supset \frac{v_1}{\sqrt{2}} e^{i\frac{a_1}{v_1}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad H_2 \supset \frac{v_2}{\sqrt{2}} e^{i\frac{a_2}{v_2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \Phi \supset \frac{1}{\sqrt{2}} e^{i\frac{a_\Phi}{v_\Phi}}, \tag{2.68}$$

where we have neglected the radial and charged modes and we choose $v_\Phi \gg v_{1,2}$ in order to decouple the scale of spontaneous PQ breaking from the EW scale. In the DFSZ model, the PQ symmetry is realised through the rephasing symmetry of the scalar sector, allowed by the interactions in its potential. The corresponding Goldstone boson from spontaneously breaking the PQ symmetry of the theory can be identified by constructing the current corresponding to the spontaneously broken PQ symmetry [150, 172]

$$j_\mu^{PQ} = -Q_\Phi \Phi^\dagger i \overleftrightarrow{\partial}_\mu \Phi - Q_1 H_1^\dagger i \overleftrightarrow{\partial}_\mu H_1 - Q_2 H_2^\dagger i \overleftrightarrow{\partial}_\mu H_2 - \sum_{\psi \in \mathrm{SM}} Q_\psi \bar{\psi} \gamma_\mu \psi, \tag{2.69}$$

where the Q_i are the PQ charges of the theory, that can be fixed from the PQ invariance of the scalar potential given the PQ charge of Φ and the requirement that the PQ current is orthogonal to the hypercharge current [150]. The axion field and its decay constant can be identified with [150]

$$a = \frac{1}{f_a} \sum_i Q_i v_i a_i, \qquad f_a^2 = \sum_i Q_i^2 v_i^2. \tag{2.70}$$

such that for $j_\mu^{PQ,a} = f_a \partial_\mu a$, the axion field is compatible with the Goldstone theorem $\langle 0 | j_\mu^{PQ,a} | a \rangle = i f_a p_\mu$. By definition, the axion does not appear in the potential. Hence, all interactions with SM particles are dictated by the Yukawa couplings. After EWSB and reexpressing the phases in the scalar doublet in terms of the axion field a, the axion-dependent Lagrangian looks as follows

$$\mathcal{L} \supset -\bar{u}_L M_u e^{iQ_1 \frac{a}{f_a}} u_R - \bar{d}_L M_d e^{iQ_2 \frac{a}{f_a}} d_R - \bar{e}_L M_e e^{iQ_2 \frac{a}{f_a}} e_R + \text{h.c.}. \tag{2.71}$$

By performing a chiral rotation on the fermion fields $\psi \to \exp(i\alpha\gamma_5)\psi$, the axion-dependent phase in front of the fermions can be removed at the cost of generating an interaction with the gauge fields

$$\begin{aligned} \mathcal{L} \supset\, & n_g \left(\frac{Q_1}{2} + \frac{Q_2}{2} \right) \frac{g_s^2}{32\pi^2} \frac{a}{f_a} G\tilde{G} + n_g \left(N_c q_u^2 Q_1 + N_c q_d^2 Q_2 + q_e^2 Q_1 \right) \frac{e^2}{32\pi^2} \frac{a}{f_a} F\tilde{F} \\ \equiv\, & N \frac{g_s^2}{32\pi^2} \frac{a}{f_a} G\tilde{G} + E \frac{e^2}{32\pi^2} \frac{a}{f_a} F\tilde{F} \end{aligned} \tag{2.72}$$

where F is the field strength of the photon field and the q_i are the electric charges of the fermions. Furthermore, in the last step we have defined the $SU(3)_c$ and $U(1)_e$ anomaly factors N and E, which in the KSVZ model take the values $N = 3$ and $E = 8$ after fixing all PQ charges.

The kinetic terms of the fermions are also not invariant under the axion-dependent chiral rotations. After performing the field redefinitions, they generate the following interactions between axions and fermions

$$\mathcal{L} \supset Q_1 \frac{\partial_\mu a}{2f_a} \bar{u}\gamma^\mu \gamma_5 u + Q_2 \frac{\partial_\mu a}{2f_a} \bar{d}\gamma^\mu \gamma_5 d + Q_2 \frac{\partial_\mu a}{2f_a} \bar{e}\gamma^\mu \gamma_5 e \,. \tag{2.73}$$

Note here, that unlike in the DFSZ model where the extra scalar was coupled to a heavy vector-like quark, in the KSVZ model the axion has tree-level couplings to the SM fermion fields at the leading order in the EFT power counting. In the KSVZ model those are only generated at the loop-level or appear at higher orders in the EFT power counting through the interactions between the axion and the vector-like quark after integrating it out.

The axion decay constant in the model is found to be [150]

$$f_a^2 = v_\Phi^2 + v^2 \sin^2 2\beta \,, \tag{2.74}$$

which again allows to arbitrarily decouple the DFSZ axion from the EW scale, as compared to Eq. (2.59) for the WW axion.

2.4.3 The EFT of Axions and Axionlike Particles

In the last two models, the axion decay constant f is decoupled from the EW scale and can become large, making the axion weakly coupled and hard to detect. Therefore, these axions have been dubbed invisible axions in the literature. In these models, the PQ symmetry is introduced by some heavy new physics at a large scale f and the axion appears as a Goldstone boson of the spontaneously breaking the symmetry, making it extremely light. Therefore, an EFT description of these models with the axion added to the light degrees of freedom is appropriate. Furthermore, in the models we just looked into, the axions do not only come with the topological coupling to gluons that is necessary to solve the strong CP problem, but also other couplings to fermions and other gauge bosons. This motivates us to define a more general class of an *axion-like particle* (ALP), that is the pseudo-Nambu–Goldstone boson (pNGB) of a spontaneously broken $U(1)$ symmetry and can have couplings to any SM particles but no longer has to solve the strong CP problem. From here on, we will call an axion, which solves the strong CP problem, a 'QCD axion' and a pNGB of a spontaneously broken $U(1)$ symmetry, which can but does not necessarily have to solve the strong CP problem, simply an 'axion' or an 'ALP'.

ALPs are ubiquitous in many BSM theories and are therefore well-motivated BSM candidates to look for. It is convenient to study them in a model-independent way by considering an EFT of the ALP together with all other SM degrees of freedom. Here, in the usual EFT spirit, the particle spectrum and the symmetries of the theory have to be taken into consideration. The particle spectrum is that of the SM extended by a real scalar transforming as a singlet under the SM gauge group but is subjected to a shift symmetry. Following the CCWZ construction [173, 174] for the pNGB[13] of the PQ symmetry. The shift symmetry is

[13]We include an explicit mass breaking the shift symmetry softly, i.e. no further shift-breaking couplings

most easily implemented by coupling the ALP derivatively to the SM fields. This yields the following Lagrangian at leading order [175]

$$\begin{aligned}\mathcal{L} =& \mathcal{L}_SM + \frac{1}{2}\partial_\mu a \partial^\mu a - \frac{m_{a,0}^2}{2}a^2 + \frac{\partial_\mu a}{f}\sum_{\psi=L,e,Q,u,d}\bar{\psi}C_\psi\gamma^\mu\psi + C_{a\tilde{G}}\frac{a}{f}G^A_{\mu\nu}\tilde{G}^{A,\mu\nu}\\ &+ C_{a\tilde{W}}\frac{a}{f}W^I_{\mu\nu}\tilde{W}^{I,\mu\nu} + C_{a\tilde{B}}\frac{a}{f}B_{\mu\nu}\tilde{B}^{\mu\nu} + \mathcal{O}\left(\frac{1}{f^2}\right)\end{aligned} \tag{2.75}$$

In this Lagrangian we have already removed a redundant coupling between the axion and Higgs bosons $\partial^\mu a\left(H^\dagger i\overleftrightarrow{D}_\mu H\right)$ by carrying out a global hypercharge transformation [175]. Furthermore, some of the derivative couplings to fermions can be removed due to the conservation of baryon number and lepton family number in the SM, which is the subgroup $U(1)^3_{L_i}\times U(1)_B$ of the flavour group of the free SM fermions $U(3)_Q\times U(3)_u\times U(3)_d\times U(3)_L\times U(3)_e$ left invariant by the SM Yukawa couplings. Due to these symmetries, there are four classically conserved currents[14]

$$\partial_\mu j^\mu_{B,L_i} = 0\,, \tag{2.76}$$

which can be used to remove some of the diagonal couplings of the derivative couplings of the ALP to fermions. One convenient choice introduced in Ref. [176] is to remove the '11' component of $\mathcal{O}_Q$ and all diagonal components of $\mathcal{O}_L$.

The generic couplings introduced in Eq. (2.75), might look familiar from the discussion of the benchmark models discussed in Sec. 2.4.2, where the interactions had more specific coefficients. This shows once again the advantage of EFTs: performing the analysis of observables in the EFT or studying features of the EFT allows us to make statements about a plethora of models (in the case of axions all the previously discussed models and many more) in a relatively model-independent way. That is why ALP EFTs have been subject to meticulous study and have been used to constrain new physics scenarios featuring axions in a model-independent way, for instance, by studying observables in flavour physics [177–191] or observables at colliders like the LHC [192–211].

It can sometimes be convenient to work in another basis, where the axion is not derivatively coupled to fermions but instead has the following couplings

$$\begin{aligned}\mathcal{L} =& \frac{1}{2}\partial_\mu a \partial^\mu a - \frac{m_{a,0}^2}{2}a^2 + C_{a\tilde{G}}\frac{a}{f}G^A_{\mu\nu}\tilde{G}^{A,\mu\nu} + C_{a\tilde{W}}\frac{a}{f}W^I_{\mu\nu}\tilde{W}^{I,\mu\nu} + C_{a\tilde{B}}\frac{a}{f}B_{\mu\nu}\tilde{B}^{\mu\nu}\\ &- \frac{a}{f}\left(\bar{Q}\tilde{Y}_u\tilde{H}u + \bar{Q}\tilde{Y}_d Hd + \bar{L}\tilde{Y}_e He + \text{h.c.}\right) + \mathcal{O}\left(\frac{1}{f^2}\right).\end{aligned} \tag{2.77}$$

This change of basis can be achieved by applying a chiral rotation on all fermions $\psi\to\psi+iC_\psi\frac{a}{f}$, where the C_ψ are the Wilson coefficients of the derivatively coupled ALP-fermion interactions in Eq. (2.75). On a first look this Lagrangian does not look shift-invariant. However, once

will be generated perturbatively, making the axion a *pseudo*-NGB.

[14] All of these symmetries are anomalous at the quantum level and hence, effectively linear combinations of the fermionic operators $\mathcal{O}_\psi$ are turned into linear combinations of bosonic operators $\mathcal{O}_{a\tilde{B}}, \mathcal{O}_{a\tilde{W}}$ coupling the ALP to gauge fields [176].

the fermionic Wilson coefficients $\tilde{Y}_{u,d,e}$ fulfil the relations [176, 194, 212, 213]

$$\tilde{Y}_e = i(Y_e C_e - C_L Y_e), \quad \tilde{Y}_{u,d} = i(Y_{u,d} C_{u,d} - C_Q Y_{u,d}), \tag{2.78}$$

the Lagrangian is shift-symmetric at the leading order in the EFT. These relations are complicated matrix relation in flavour space, depending on five generic hermitian matrices. Hence in Chap. 6, we will make an effort in recasting these relations into simple algebraic relations that allow to clearly implement the power countings of the shift-symmetric and shift-breaking sectors of the EFT, which clearly is not possible in the form of Eq. (2.78).

Furthermore, it is an important task to systematically construct an operator basis beyond the leading order in Eq. (2.75) and find the conditions of the form of Eq. (2.78), that encode shift symmetry beyond the leading order in the EFT. We will perform this task in Chap. 7 and will introduce an important tool for the construction of an operator basis in the following section.

2.5 Group Invariants and the Hilbert Series

Physics and particle physics in particular is heavily based on the use of symmetries to reduce unphysical degrees of freedom to an efficient description of nature. Hence, a prevalent task in theoretical physics is to find objects which are invariant under the action of a group. Due to the restrictiveness of the symmetries used, it is often possible to perform this task by brute force by exhausting all possible contractions among objects transforming under a given group. However, in more complicated theories where objects transform in involved representations, the symmetry group is very complex or when the number of objects (and their allowed combinations) that transform under the group grows, this task can become increasingly difficult.

For this reason, physicists have started to borrow tools from mathematical invariant theory [64, 214–216] that take care of this counting task for EFT operator bases, i.e. invariants under Poincaré and gauge symmetry, as well as with the EOM and IBP redundancies removed, and invariants under internal symmetries, like flavour invariants.

The problem at hand is the following. Given a set of parameters x that transform in the representation R of a group $\mathcal{G}$

$$x \to x' = R(g)x, \; g \in \mathcal{G}, \tag{2.79}$$

an invariant I is defined as a combination of these parameters which does not transform under the action of the symmetry

$$\mathcal{I}(x) \overset{\mathcal{G}}{\to} \mathcal{I}(x') = \mathcal{I}(x). \tag{2.80}$$

The task is to count how many independent invariants, that can be formed from the set of parameters, exist. To be more concrete, let us start with a simple example. Let ϕ be a complex field transforming under a $U(1)$ symmetry

$$\phi \to e^{i\alpha}\phi. \tag{2.81}$$

It is a simple exercise to construct all possible invariants of ϕ under this $U(1)$ symmetry, by noticing that the combination

$$\mathcal{I} = \phi\phi^* \tag{2.82}$$

is invariant. All other invariants are just powers of this simple invariant and we can define a generating functional of the invariants

$$1 + \mathcal{I} + \mathcal{I}^2 + \mathcal{I}^3 + \cdots = \frac{1}{1 - \mathcal{I}}, \tag{2.83}$$

that counts all invariants that can be built out of ϕ. Eq. (2.83) is the so-called Hilbert series of the theory. For more complicated theories where it is hard to keep track or even construct all possible invariants under a given group, the Hilbert series will become invaluable in counting all possible invariants that can be built from combinations of the objects transforming under a given group. The question is how to compute the Hilbert series efficiently and how to interpret its form. We will discuss this in more detail below.

There are two scenarios we have in mind here. The first one is the counting and construction of flavour invariants that are made of tensors transforming under some symmetry group. These kind of invariants only have algebraic redundancies among them complicating the counting of the non-redundant ones. The other slightly more complicated case is that of finding an operator basis for EFTs. Finding an operator basis for on-shell computations, which is finding invariants under the gauge and Poincaré group, is complicated by the existence of IBP and EOM redundancies discussed in Sec. 2.5.2. These highly non-trivial constraints call for more theoretical effort expanding the Hilbert series used for Lie groups to remove these additional redundancies.

2.5.1 Invariants Under Internal Symmetries

As introduced earlier, one important task in particle theory is to find the invariants under the action of internal symmetry groups, which for our purposes are always Lie groups. There exist some useful definitions and language in the literature to organise the construction of invariants. We will introduce them here along with some important results from invariant theory, mostly following Refs. [64, 217–220]. Some of the material presented here has also appeared in Ref. [4].

One important class of such symmetries are approximate symmetries of a Lagrangian which become exact in the limit of some vanishing Lagrangian parameter. Such softly broken symmetries can be formally reinstated in the Lagrangian even in the presence of the breaking parameters. This is done by promoting the breaking couplings to fields and making them transform under the symmetry, such that the Lagrangian is formally invariant under the action of the symmetry. The parameters are said to transform spuriously under the symmetry and are often called spurions. At the end, the spurion fields receive a VEV corresponding to their physical value, allowing to systematically take into account the breaking effects of the symmetry. A theory that only contains couplings which increase the exact symmetries of the theory when being sent to zero, is called technically natural [221]. As a result, any correction of the parameter must again be proportional to the parameter, such that the symmetry is

	$U(3)_Q$	$U(3)_u$	$U(3)_d$	$U(3)_L$	$U(3)_e$
Y_u	$\mathbf{3}_{+1}$	$\bar{\mathbf{3}}_{-1}$	$\mathbf{1}_0$	$\mathbf{1}_0$	$\mathbf{1}_0$
Y_d	$\mathbf{3}_{+1}$	$\mathbf{1}_0$	$\bar{\mathbf{3}}_{-1}$	$\mathbf{1}_0$	$\mathbf{1}_0$
Y_e	$\mathbf{1}_0$	$\mathbf{1}_0$	$\mathbf{1}_0$	$\mathbf{3}_{+1}$	$\bar{\mathbf{3}}_{-1}$

Table 2.2: Spurionic transformation behaviour of the SM Yukawa couplings $Y_{u,d,e}$ under $U(3)^5$, the largest flavour group allowed by the kinetic term of the SM fermions. The subscripts of the $SU(3)$ representations denote the charge under the $U(1)$ part of the flavour symmetry.

still preserved in the limit of taking the coupling to zero.

One example for such a symmetry are flavour symmetries in the SM. Taking the SM Lagrangian in Eq. (2.1), one can recognise that the SM Lagrangian has an exact $U(3)_Q \times U(3)_u \times U(3)_d \times U(3)_L \times U(3)_e$ flavour symmetry, when $Y_{u,d,e} \to 0$. This symmetry can be reinstated in the presence of finite Yukawa couplings, by letting the SM Yukawa couplings transform as indicated in Tab. 2.2 under $U(3)^5$.[15] One interesting question is, what are the invariant objects one can built from these transforming building blocks. This will for instance give us a basis independent measure for CP violation in the SM, the Jarlskog invariant that was introduced earlier.

At this point it is useful to introduce some notation and jargon commonly used in the invariant literature. As flavour invariants are polynomials of the parameters in the theory, not all possible invariants that can be built from the flavourful couplings in the theory will be independent. One useful definition is the one of the *generating* or *basic* set of invariants, which is a minimal set of invariants that allows to express all other invariants in the theory as a polynomial of them. This set always has finite cardinality for reductive groups [217, 219]. If any invariant can be expressed as a polynomial of the invariants in the generating set, we will call that relation an *explicit relation*. This is opposed to the polynomial relations that still exist among the generating invariants. Indeed, the generating set may still be *algebraically dependent* and there can exist relations of the form

$$P\left(\mathcal{I}_1, \ldots, \mathcal{I}_m\right) = 0\,, \tag{2.84}$$

referred to as *syzygies* in the invariant literature.

Among the set of generating invariants, there exists a set of invariants that are *algebraically independent*, the so-called *primary invariants*. Their algebraic independence implies that there exist no syzygies among only the primary invariants. A non-trivial result is that the number of physical parameters, i.e., the minimal number of parameters that are left after all transformations allowed by the symmetry group of the theory are used, is equal to the number of invariants in the primary set [217–219].

Information about all of these invariants is encoded in the Hilbert series, which we now

[15]This is also an example of a technically natural coupling. When the Yukawa couplings go to zero, the Lagrangian has a $U(3)^5$ chiral symmetry. Therefore, corrections to the Yukawa couplings in the SM must again be proportional to Yukawa couplings, keeping the corrections small.

define more carefully as

$$\mathcal{H}(q) = \sum_{i=0}^{\infty} c_i q^i \,, \tag{2.85}$$

where c_i is the number of invariants that can be built from the given set of building blocks labelled by the parameter q at a given order i. One important property of the Hilbert series is that it can always be written as a fraction of two polynomials [219][16]

$$\mathcal{H}(q) = \frac{\mathcal{N}(q)}{\mathcal{D}(q)} \,. \tag{2.86}$$

The numerator and denominator come in a special form. The numerator is palindromic, i.e. $\mathcal{N}(q) = t^p \mathcal{N}(1/q)$, where p is the highest power of q in $\mathcal{N}(q)$ and all terms in $\mathcal{N}(q)$ come with a positive sign. The denominator is of the form $\mathcal{D}(q) = \prod_{i=1}^{m}(1 - q^{d_i})$, where m counts the total number of factors in the denominator and d_i gives the total power of spurions in the invariant. It can be shown that each of the factors in the denominator corresponds to an invariant in the primary set [217–219]. Furthermore, for a trivial numerator, i.e. $\mathcal{N}(q) = 1$, the generating set is equivalent to the primary set and the ring is called a *free ring*.

The Hilbert series can be straightforwardly generalised to a theory with several different couplings. In a theory with n couplings the Hilbert series is defined as

$$\mathcal{H}(q_1, \ldots, q_n) = \sum_{i_1=0}^{\infty} \cdots \sum_{i_n=0}^{\infty} c_{i_1 \ldots i_n} q_1^{i_1} \ldots q_n^{i_n} \,, \tag{2.87}$$

where the coefficient $c_{i_1 \ldots i_n}$ now counts the number of invariants containing the spurions $(q_1, \ldots, q_n)$ to the power $(i_1, \ldots, i_n)$. The multi-graded Hilbert series is no longer guaranteed to come in the form of Eq. (2.86) with a palindromic numerator with positive terms and the denominator counting the number of primary invariants. This information can still be retrieved by taking the single-graded limit of the Hilbert series, $\mathcal{H}(q_1, \ldots, q_n) \to \mathcal{H}(q, \ldots, q)$.

From the discussion up to here, it is not clear how to compute the Hilbert series. One practical way to compute the Hilbert series for reductive Lie groups is the Molien-Weyl formula, which for a single coupling transforming in the representation R of the group G is defined as

$$\mathcal{H}(q) = \int d\mu_G \; \exp\left(\sum_{k=1}^{\infty} \frac{q^k \chi_R\left(z_1^k, \ldots, z_d^k\right)}{k} \right) \equiv \int d\mu_G \; \mathrm{PE}\left[\chi_R(z_1, \ldots, z_d); q\right] . \tag{2.88}$$

Here, $d\mu_G$ is the Haar measure of the group, $\chi_R(z_1, \ldots, z_d) = \mathrm{Tr}\left(g(z_1, \ldots, z_d)\right)$ is the character of the representation R of the group G of rank d, defined as the trace over a group element $g \in G$, and we have defined the *plethystic exponential* in the last step. Even though this formula looks complicated, there is a simple interpretation of it. The characters of compact

[16] Strictly speaking, this is only true when the polynomial ring of the flavour invariants is Cohen-Macaulay, which is the case for the flavour invariant rings studied in this thesis.

Lie groups are orthonormal with respect to integration of the Haar measure of the group

$$\int d\mu_G\,(z_1,\ldots,z_d)\ \chi_R\,(z_1,\ldots,z_d)\,\chi^*_{R'}\,(z_1,\ldots,z_d) = \delta_{R,R'}\,. \tag{2.89}$$

To achieve our goal of finding all invariants of a group, we can simply use this property to project onto the singlet representation of the group, i.e. plugging $\chi^*_{R'} = 1$ into Eq. (2.89). The left-over task is to construct all possible combinations of characters capturing all possible tensor products of the representations of the building blocks. This is exactly what the plethystic exponential does. Hence, the integration over the Haar measure simply projects out all the invariant combinations of representations defined by the transforming parameters of the theory, that are generated by the plethystic exponential, yielding all singlets under the group. The Molien-Weyl formula can be generalised for a theory with several couplings transforming in different representations R_i

$$\mathcal{H}(q_1,\ldots,q_n) = \int d\mu_G \prod_{i=1}^{n} \mathrm{PE}\left[\chi_{R_i}(z_1,\ldots,z_d);q_i\right]. \tag{2.90}$$

To compute the characters and Haar measures of the Lie groups in this thesis, we will make use of the maximal torus of the groups. For a connected Lie group G, like $U(N)$, any $g \in G$ can be expressed as an element of the maximal torus $T = U(1)^{\mathrm{rank(G)}}$, i.e. $\exists h \in G : h^{-1}gh \in T$ [64, 222]. In the following, we will mostly work with the group $U(N)$. Let us derive the character for $U(3)$ as an example. Following what we have just discussed, the maximal torus of $U(3)$ is $U(1)^3$ and a matrix representation will have the following form [222]

$$\mathrm{diag}\left(e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3}\right), \quad \theta_{1,2,3} \in \mathbb{R}\,. \tag{2.91}$$

We can define $z_n = e^{i\theta_n}$, which are the parameters of the maximal torus integrated over in the Molien–Weyl formula. Then, the character of the fundamental of $U(3)$ is simply

$$\chi^{\mathbf{3}}_{U(3)} = \mathrm{Tr}\,\mathrm{diag}\,(z_1,z_2,z_3) = z_1 + z_2 + z_3\,, \tag{2.92}$$

and similarly we find for the character of the conjugate representation

$$\chi^{\bar{\mathbf{3}}}_{U(3)} = \mathrm{Tr}\,\mathrm{diag}\left(z_1^{-1}, z_2^{-1}, z_3^{-1}\right) = z_1^{-1} + z_2^{-1} + z_3^{-1}\,. \tag{2.93}$$

The corresponding Haar measure can be found in Ref. [64], which together with the explicit form of the character will allow us to compute the Hilbert series by solving the integral in the Molien–Weyl formula.

Another useful function is the so-called plethystic logarithm, which is the inverse function of the plethystic exponential that we have just defined, i.e., $\mathrm{PE}^{-1}(f(x)) = \mathrm{PL}(f(x))$ and is defined as follows

$$\mathrm{PL}\left[f\,(x_1,\ldots,x_N)\right] = \sum_{n=1}^{\infty} \frac{\mu(n)}{n} \log\left[f\,(x_1^n,\ldots,x_N^n)\right], \tag{2.94}$$

where $\mu(n)$ is the Möbius function defined as

$$\mu(n) = \begin{cases} 0 & n \text{ has repeated prime factors} \\ 1 & n = 1 \\ (-1)^j & n \text{ is product of } j \text{ distinct prime numbers} \end{cases} . \tag{2.95}$$

For concreteness and for later reference, we will discuss the construction of the invariants of the SM Yukawa couplings with the help of the Hilbert series here, which has first been achieved in Ref. [218]. We have just computed the characters of the representations the building blocks transform under (c.f. Tab. 2.2). Together, with the Haar measure found in Ref. [64] we can evaluate the Molien–Weyl formula in Eq. (2.90) and solve the integrals by making use of the residue theorem. We find for the Hilbert series of the SM Yukawa couplings

$$\begin{aligned} \mathcal{H}(e,u,d) =& \frac{1+u^6d^6}{(1-e^2)(1-e^4)(1-e^6)(1-u^2)(1-u^4)(1-u^6)(1-d^2)(1-d^4)(1-d^6)} \times \\ & \times \frac{1}{(1-u^2d^2)(1-u^4d^2)(1-u^2d^4)(1-u^4d^4)} . \end{aligned} \tag{2.96}$$

From the denominator of the Hilbert series, one can read off that there exist in total 13 primary invariants. These correspond to the three charged lepton masses and the six masses of the quarks, as well as the three mixing angles and the phase in the CKM matrix. One can furthermore observe, that the algebraic structure of the lepton sector invariants are those of a free ring, while the numerator of the Hilbert series shows that there exists one further invariant in the quark sector of the SM at the order $Y_u^6 Y_d^6$ in the quark Yukawa couplings, which must have a syzygy at the squared order, since this is the only term appearing in the numerator of the Hilbert series. Constructing these invariants explicitly, one finds [218]

$$\mathrm{Tr}\left(X_e\right), \quad \mathrm{Tr}\left(X_e^2\right), \quad \mathrm{Tr}\left(X_e^3\right) \tag{2.97}$$

in the lepton sector and

$$\begin{aligned} &\mathrm{Tr}\left(X_u\right), \quad \mathrm{Tr}\left(X_u^2\right), \quad \mathrm{Tr}\left(X_u^3\right), \mathrm{Tr}\left(X_d\right), \quad \mathrm{Tr}\left(X_d^2\right), \quad \mathrm{Tr}\left(X_d^3\right) \\ &\mathrm{Tr}\left(X_u X_d\right), \quad \mathrm{Tr}\left(X_u^2 X_d\right), \quad \mathrm{Tr}\left(X_u X_d^2\right), \quad \mathrm{Tr}\left(X_u^2 X_d^2\right) \end{aligned} \tag{2.98}$$

in the quark sector for the primary set of invariants, capturing the magnitude of all parameters in the SM Yukawa couplings. The additional invariant at order $Y_u^6 Y_d^6$ is the Jarlskog invariant

$$J_4 = \mathrm{Im}\,\mathrm{Tr}\left(\left[X_u, X_d\right]^3\right) , \tag{2.99}$$

which only captures the sign information of the CKM phase [218]. This is compatible with the fact that there exists a syzygy of the Jarlskog invariant allowing to express its square J_4^2 in terms of the primary quark invariants. Therefore, only the Jarlskog invariant itself but not its square can contain physical information [218]. We can also compute the plethystic logarithm of the SM flavour invariants. We find,

$$\mathrm{PL}(u,d,e) = e^2+e^4+e^6+u^2+u^4+u^6+d^2+d^4+d^6+u^2d^2+u^4d^2+u^2d^4+u^4d^4+u^6d^6-u^{12}d^{12} \tag{2.100}$$

Here, one helpful property of the plethystic logarithm is apparent: One can simply read off the number of generating invariants and the syzygies among them from the coefficients of the terms in the plethystic logarithm. Here, the positive terms correspond to generating invariants and the negative terms correspond to the syzygies among them [223, 224].

The plethystic logarithm is not always as simple in the SM. Indeed, the plethystic logarithm is only a finite polynomial with the above interpretation of the terms, if the underlying ring has the structure of a *complete intersection ring*. This is the case when the difference in the number of generating invariants and the number of syzygies is equal to the number of algebraically independent invariants; otherwise it is called a *non-complete intersection ring* [219, 220]. In a non-complete intersection ring the terms have to be interpreted slightly differently. There, the *leading positive* terms, i.e., all positive terms up to the first term with a negative sign in the plethystic logarithm, can be identified with the basic invariants, while the *leading negative*, i.e., the first negative terms that appear after the leading positive terms, correspond to the syzygies.

We also want to note here that in more complicated rings, the regions where positive and negative terms appear are no longer necessarily as well-separated as in what we have discussed up to here. We will see in Chap. 3 that in theories with more complicated representations or symmetry groups, the interpretation of the positive and negative terms in the plethystic logarithm have to be slightly changed, where the coefficient of each term in the plethystic logarithm should count the difference between the number of generating invariants and the number of syzygies among the generating invariants instead [4, 220].

2.5.2 Invariants for EFT Operator Bases

Another case where the counting of invariants becomes complicated quickly is in the case of operator bases for EFT operators. What complicates matters further is the fact that the invariants, that can be formed under the Poincaré and gauge group, the EFT is based on, do not yield a minimal operators basis. In particular, the EOM and IBP redundancies discussed in Sec. 2.2.1 are still present in the counting if the previously shown form of the Hilbert series is applied. Furthermore, the Lorentz group $SO(3,1)$ in Minkowski space is a non-compact group, meaning that the orthonormality condition of the characters can no longer be utilised to project onto the singlet of the group. In order to correctly count the operators in an EFT operator basis with all these redundancies removed, some further steps have to be applied. In this section, we will briefly review all the required machinery to address these issues following Refs. [64, 85, 215, 225, 226]. Some of the material presented here has also appeared in Ref. [2].

For the construction of an operator basis for EFTs, the basic logic behind the Hilbert series is the same as for the construction of flavour invariants: we want to find invariants under the action of the Poincaré and gauge group for a given number of fields and derivatives transforming under these groups. Denoting the field spurions as $\{\phi_i\}$ and and the derivative spurion as $\mathcal{D}$, we can schematically write the Hilbert series as

$$\mathcal{H}(\mathcal{D},\{\phi_i\}) = \sum_{r_1,\dots,r_n} \sum_k c_{\mathbf{r}\,k}\, \phi_1^{r_1} \dots \phi_n^{r_n} \mathcal{D}^k, \tag{2.101}$$

where $c_{\mathbf{r}\,k} \equiv c_{r_1,\dots,r_n,k}$ counts the number of independent operators with k derivatives $\mathcal{D}$ and r_i fields ϕ_i.

As before, the Hilbert series can be computed from the Molien-Weyl formula, based on the fact that the characters are orthogonal with respect to the integration over the Haar measure of the group and using the plethystic exponential as a generating functional of all possible tensor products of representations that can be built in the theory. Due to the different spin statistics of fermions and bosons, the plethystic logarithm only has to be slightly modified [64, 214]

$$\mathrm{PE}\left[\phi_{\mathbf{R}}\,\chi_{\mathbf{R}}(z)\right] = \exp\left(\sum_{r=1}^{\infty} \frac{1}{r} (\pm 1)^{r+1} \phi_{\mathbf{R}}^r\, \chi_{\mathbf{R}}(z^r)\right), \tag{2.102}$$

where the spurions of the fermionic fields receive the additional minus sign. As for the flavour invariants in a theory with several couplings, the full plethystic exponential is defined as the product of the plethystic exponentials of the fields $\mathrm{PE}[\{\phi_i\}] = \prod_i \mathrm{PE}[\phi_i]$ without showing characters explicitly.

The situation becomes more involved with the additional constraints that have to be imposed on the Poincaré and gauge invariants due to EOM and IBP redundancies mentioned in Sec. 2.2.1. It was found in Ref. [64], that the representations of the conformal group can be used to address these issues. We will briefly sketch the idea here with the example of a scalar field and refer the reader to Ref. [64] for a detailed discussion.

In QFT, we work with local fields, that interpolate between a single particle state excited by the field and the vacuum. The first observation we want to make is about which objects built from a single scalar field can appear in a correlator between a single particle state and the vacuum. Due to Wigner's classification of representations of the Lorentz group, a single particle state of a massive scalar ϕ can be specified by its mass $p^2 = m^2$, its spin (which is just zero) and additional quantum numbers σ. We denote this state by $|\mathbf{p}\rangle$ here, suppressing the potential dependence on other quantum numbers. Then, the interpolating fields between this state and the vacuum are [64]

$$\begin{aligned} \langle 0|\phi|\mathbf{p}\rangle &\sim e^{-ip\cdot x} \\ \langle 0|\partial_\mu\phi|\mathbf{p}\rangle &\sim p_\mu e^{-ip\cdot x} \\ \langle 0|\partial_{\{\mu_1}\partial_{\mu_2\}}\phi|\mathbf{p}\rangle &\sim p_{\{\mu_1}p_{\mu_2\}} e^{-ip\cdot x} \\ &\vdots \end{aligned}\quad, \tag{2.103}$$

where the traceless and anti-symmetric components have been removed. The trace component is just $p^2 = m^2$, simply reducing derivatives of the field to the field itself, and the anti-symmetric component vanishes trivially. Motivated by this, we define the single-particle module of the scalar field

$$R_\phi = \begin{pmatrix} \phi \\ \partial_{\mu_1}\phi \\ \partial_{\{\mu_1}\partial_{\mu_2\}}\phi \\ \vdots \end{pmatrix}, \tag{2.104}$$

and similar modules can be defined for fermion and vector fields. The next step is to implement these building blocks into a character of a group, so they can be used in the Hilbert series to construct singlets of the group. It turns out that these modules can be identified with the representations of the conformal group $SL(2,\mathbb{C}) \cong SU(2) \times SU(2)$.

Using the state-operator correspondence of conformal field theories, we can organise operators into irreducible representation of the conformal group. These representations have the following form

$$R_{[\Delta,l]} = \begin{pmatrix} \mathcal{O}_l \\ \partial_{\mu_1}\mathcal{O}_l \\ \partial_{\mu_1}\partial_{\mu_2}\mathcal{O}_l \\ \vdots \end{pmatrix}, \tag{2.105}$$

where $\mathcal{O}_l$ is some operator, which we will call primary, of spin l and scaling dimension Δ and the remaining components are called the descendants of $\mathcal{O}_l$. The conformal representation $R_{[\Delta,l]}$ is reminiscent of the 1-particle module we have defined in Eq. (2.104).

To build operators containing several (different) fields, we will use tensor products of the single particle modules to build all possible Lorentz invariant operators from the fields

$$\begin{pmatrix} \phi \\ \partial_{\mu_1}\phi \\ \partial_{\{\mu_1}\partial_{\mu_2\}}\phi \\ \vdots \end{pmatrix}^{\otimes n} \sim \sum_{\mathcal{O}} \begin{pmatrix} \mathcal{O} \\ \partial\mathcal{O} \\ \partial^2\mathcal{O} \\ \vdots \end{pmatrix}. \tag{2.106}$$

Then, as for the flavour invariants, we can use conformal representation theory to project out the singlets under the conformal group which correspond to the first entry in the tensor product of the single particle modules. As for the flavour invariants, we will define plethystic exponentials as generating functionals for the single particle modules in order to generate all possible tensor products of the given fields and its descendants. The characters appearing in the generating functionals of the representations of the conformal group are [64][17]

$$\chi_{[\Delta,l]}(\mathcal{D};x) = \sum_{n=0}^{\infty} \mathcal{D}^{\Delta+n}\chi_{\mathrm{Sym}^n(\frac{1}{2},\frac{1}{2})}(x)\chi_l(x) = \mathcal{D}^{\Delta}\chi_l(x)P(\mathcal{D},x) \tag{2.107}$$

[17] Here, only the symmetric tensor product of derivatives (c.f. $\mathrm{Sym}^n(\frac{1}{2},\frac{1}{2})$) is considered, because the anti-symmetric part simply yields the field strength of the gauge fields appearing in the covariant derivative, which are taken into account separately.

for a primary operator transforming in the representation $R_{[\Delta,l]}$ under the conformal group. Here, $\mathcal{D}$ denotes the derivative spurion living in the $\left(\frac{1}{2},\frac{1}{2}\right)$ representation of the Lorentz group,[18] $\chi_l(x)$ is the character of the spin l representation of $SO(4)$ and x are the coordinates of the maximal torus representation of the conformal group $SL(2,\mathbb{C})$. In the last step we have defined the generating function of symmetric products of the vector representation

$$P(\mathcal{D},x) = \sum_{n=0}^{\infty} \mathcal{D}^n \chi_{\mathrm{Sym}^n\left(\frac{1}{2},\frac{1}{2}\right)}(x) = \frac{1}{(1-\mathcal{D}x_1)(1-\mathcal{D}x_1^{-1})(1-\mathcal{D}x_2)(1-\mathcal{D}x_2^{-1})}\,, \tag{2.108}$$

which will frequently appear later. One can intuitively understand the character formula by looking at the form of the conformal representation. The descendants are generated by successively applying derivatives to the primary operator. This is exactly what is summed over in Eq. (2.108). The first term in the sum corresponds to the primary operator, the second term corresponds to one derivative applied to the primary operator and so on. P as the generating function of symmetric products of the vector representation can be understood as the generator of the descendants of a primary operator.

The character for the single-particle module of a scalar ϕ presented in Eq. (2.104) with spin $l=0$ and scaling dimension $\Delta=1$ according to Eq. (2.108) then simply reads

$$\chi_{[1,0]}(\mathcal{D};x) = \mathcal{D}P(\mathcal{D},x)\,. \tag{2.109}$$

The character for fermion and vector fields can be obtained in a similar fashion from Eq. (2.108). This will allow us to construct all possible Lorentz and gauge invariant operators. The next step is to address the redundancies introduced by IBP and the EOM, which as it turns out can also be done using conformal representation theory. For definiteness we will continue discussing the EOM and IBP redundancies with the example of a scalar field.

EOM Redundancies To remove EOM redundancies in the Hilbert series construction, we have to find a way to remove terms of the form $\{\partial^2\phi, \partial_{\mu_1}\partial^2\phi, \dots\}$ from the single particle module of the scalar (and similar terms for fermion and vector fields, see Ref. [64]) by the help of conformal characters.

We have already done this earlier in the single-particle module, when removing the $p^2=m^2$ pieces, which are exactly the pieces which are redundant by the EOM on-shell. In order to implement this for the Hilbert series, we have to find a way of removing the corresponding entries from the conformal character. This is done by a so-called shortening condition to the character, which exactly removes the EOM-redundant pieces. To remove the EOM-redundant terms, we simply have to remove all the terms where two derivatives are contracted from the character of the full conformal character of the scalar. This is achieved by applying the following shortening condition to the character of the full conformal representation of the

[18] Note that the Lorentz group is non-compact, and its characters are not orthonormal, making it incompatible with the orthonormality condition that is used in the Molien-Weyl formula to compute the Hilbert series. Therefore, we will work in Euclidean space, where the Lorentz group $SO(4)$ is isomorphic to $[SU(2)_L \otimes SU(2)_R]/Z_2$, which is compact and has orthonormal characters. The covariant derivative $\mathcal{D}$ transforms in the fundamental $\left(\frac{1}{2},\frac{1}{2}\right)$ representation of $[SU(2)_L \otimes SU(2)_R]/Z_2$.

scalar introduced in Eq. (2.109)

$$\chi_\phi(\mathcal{D};x) = \sum_{n=0}^{\infty} \mathcal{D}^{n+d_a} \chi_{\mathrm{Sym}^n(\frac{1}{2},\frac{1}{2})}(x) - \sum_{n=2}^{\infty} \mathcal{D}^{n+d_a} \chi_{\mathrm{Sym}^{n-2}(\frac{1}{2},\frac{1}{2})}(x) = \mathcal{D}\left(1-\mathcal{D}^2\right) P(\mathcal{D},x)\,, \quad (2.110)$$

which now has all EOM-redundant terms removed. This formula can again be understood intuitively. The only way to raise the scaling dimension of an operator while keeping its its spin structure the same is to add contracted derivatives. Therefore, the second term in Eq. (2.110) exactly removes a term which has the same scaling dimension as the previous operator but two derivatives less in the symmetric tensor product of derivatives. These are exactly the EOM-redundant terms for a scalar that we wanted to remove for each entry in the conformal representation of the scalar. The EOM redundancy for fermion and vector fields can be removed in a similar fashion. The next step is to remove the IBP redundancies.

IBP Redundancies We have to take special care to correctly remove IBP redundancies from the Hilbert series counting. Once again, we can make use of the power of conformal representation theory to get rid of the redundancies, for which we will only give hand-wavy arguments here and leave the detailed explanation to Ref. [64].

The removal of IBP redundant operators relies on the fact that the tensor product of all traceless single-particle modules, which are generated by the plethystic exponentials to construct all possible EOM-reduced operators, can again be organised in the form of conformal primary operators and their descendants

$$\begin{pmatrix} O_l \\ \partial O_l \\ \partial^2 O_l \\ \vdots \end{pmatrix}^{\otimes n} \sim \sum_{\mathcal{O}'} \begin{pmatrix} \mathcal{O}' \\ \partial \mathcal{O}' \\ \partial^2 \mathcal{O}' \\ \vdots \end{pmatrix}. \quad (2.111)$$

It turns out that the scalar primaries that appear after reorganising the tensor product of all traceless single-particle modules, are exactly the independent operators with all IBP and EOM redundancies removed. Hence, the task of removing the IBP redundancies changes to removing the descendants of the scalar primaries. But we know how the descendants of a primary operator are generated: by repeatedly applying derivatives on the primary, which is done by the generating functional P, which generates symmetric tensor products of derivatives. Therefore, removing the descendants simply amounts to inverting the action of the generating functional P on the tower of descendants. For the Hilbert series, this has the consequence that the plethystic exponential of all representations of fields, which generate all possible operators as the tensor products of the single particle modules, has to be multiplied by $1/P$.

The Hilbert Series without EOM and IBP Redundancies The final expression of the Hilbert series can be organised as follows

$$\mathcal{H}(\mathcal{D},\{\phi_i\}) = \int d\mu_{\text{Lorentz}} \int d\mu_{\text{gauge}} \frac{1}{P} \prod_i \text{PE}\left[\frac{\phi_i}{\mathcal{D}^{d_i}}\chi_i\right] + \Delta\mathcal{H}(\mathcal{D},\{\phi_i\}), \tag{2.112}$$

where $\{\phi_i\}$ corresponds to all spurions in the theory, and the character χ_i should be understood as the character of the single particle module R_{ϕ_i}. The conformal characters of R_{ϕ_i} are weighted with the scaling dimension d_i, therefore, each spurion ϕ_i in the plethystic exponential comes with $\mathcal{D}^{-d_i}$. Note here, that the second term in Eq. (2.112) appears due to a subtlety in using the conformal characters to remove the EOM redundancies. While the characters corresponding to the ordinary representations of the conformal group have some notion of orthonormality, this is no longer true after applying the shortening conditions on them that removes the EOM-redundant terms [64]. This can be understood by observing that Eq. (2.110) is a linear combination of the character of the ordinary conformal representations, hence the shortened characters no longer have to be orthonormal. This is taken care of by the term $\Delta\mathcal{H}$ in Eq. (2.112), which can be computed for any EFT given its expression in Ref. [64]. For the Hilbert series of EFT operators these terms are usually irrelevant because they just appear at mass dimension 4. As we will see in Sec. 7.3.1, if there exist some field spurions with an unusual power counting, this can change.

In order to calculate the Hilbert series defined in Eq. (2.112), the conformal characters for different fields implemented in their single particle modules, as well as the Haar measures for the different groups appearing in the EFT construction are needed. The characters for the most important representations under the conformal group as well as the characters for the representations and the Haar measures of the most common Lie groups used in particle physics can be found in Refs. [64, 85].

***C* and *P* transformations** Because the CP symmetry is a main subject of study of this thesis, we will also introduce here a way to count operators separately, which have different transformation properties under CP. The inclusion of CP into the Hilbert series has first been discussed in Ref. [64] and subsequently used in studies of various theories [105, 227, 228]. Here, we will present an overview of the necessary ingredients for integrating CP into the Hilbert series framework.

C and P transformations can be understood as transformations on the representations of the Lorentz and gauge group. Hence, they are symmetries of symmetries and effectively split the Lorentz group and gauge group into two disconnected groups

$$\begin{aligned}\widetilde{\text{Lorentz}} &= \text{Lorentz} \rtimes \Gamma_{\mathcal{P}} = \{\text{Lorentz},\ \text{Lorentz} \rtimes \mathcal{P}\} \equiv \{\widetilde{\text{Lorentz}}_+,\ \widetilde{\text{Lorentz}}_-\}, \\ \widetilde{\text{gauge}} &= \text{gauge} \rtimes \Gamma_{\mathcal{C}} = \{\text{gauge},\ \text{gauge} \rtimes \mathcal{C}\} \equiv \{\widetilde{\text{gauge}}_+,\ \widetilde{\text{gauge}}_-\},\end{aligned} \tag{2.113}$$

where $\Gamma_X = \{\mathbb{1}, X\}$ are the elements of the parity groups. In order to count all operators transforming even and odd under CP, we require building blocks with definite CP transformation under the two branches of the symmetry group we just defined. This is not the case for the SM fields, that are among the degrees of freedom appearing in the EFTs of interest later.[19] For instance, the left-handed quark doublet Q transforms into its conjugate $Q^\dagger$ under a CP transformation. Therefore, following Ref. [105], for any field spurion ϕ we will use the combination $\check{\phi} = \phi \oplus \phi^\dagger$ as building blocks in the Hilbert series. Then CP-even operators $\mathcal{O} + \mathcal{O}^{\rm CP}$ and CP-odd operators $\mathcal{O} - \mathcal{O}^{\rm CP}$ are both counted by the same operator $\check{\mathcal{O}}$, made from the new building block $\check{\phi}$.

The invariants of the two branches of the symmetry group split by CP can be counted by two Hilbert series, which are slight modifications of the Hilbert series we have presented in Eq. (2.112) to account for the CP transformations. The Hilbert series of the two branches read as follows [64][20]

$$\mathcal{H}_+(\mathcal{D}, \{\check{\phi}_i\}) = \int d\mu_{\widetilde{\text{Lorentz}}_+}(x) \int d\mu_{\widetilde{\text{gauge}}_+}(z) \frac{1}{P_+(\mathcal{D}, x)} \prod_i \text{PE}\left[\frac{\check{\phi}_i}{\mathcal{D}^{d_i}} \chi_i^+(\mathcal{D}, x, z)\right], \quad (2.114)$$

$$\mathcal{H}_-(\mathcal{D}, \{\check{\phi}_i\}) = \int d\mu_{\widetilde{\text{Lorentz}}_-}(\tilde{x}) \int d\mu_{\widetilde{\text{gauge}}_-}(\tilde{z}) \frac{1}{P_-(\mathcal{D}, \tilde{x})} \prod_i \text{PE}'\left[\frac{\check{\phi}_i}{\mathcal{D}^{d_i}} \chi_i^-(\mathcal{D}, x, z)\right], \quad (2.115)$$

where $x \equiv (x_1, x_2)$ parameterises the Lorentz group and $z \equiv (z_{c,1}, z_{c,2}, z_W, z_Y)$ are the parameters of the SM gauge groups $\text{SU}(3)_c \times \text{SU}(2)_W \times \text{U}(1)_Y$. The Hilbert series $\mathcal{H}_+$ counts the invariants under the action of the group $SO(4) \times SU(3) \times SU(2) \times U(1)$, while $\mathcal{H}_-$ counts the invariants under the action of the parity-transformed group $(SO(4) \times SU(3) \times SU(2) \times U(1)) \rtimes \mathcal{CP}$.

The characters $\chi_i^\pm$ in the two branches of the Hilbert series can be obtained from those previously shown. In particular, the character χ^+ of the newly defined spurion $\check{\phi}$ is given by the sum of the characters of the spurion and its conjugate. In addition, since the plus branch of the gauge and Lorentz group is the part of the group which is unchanged by C and P transformations, the group measures and momentum generating functional P_+ of $\mathcal{H}_+$ are the same as those of the full Hilbert series $\mathcal{H}$. On the other hand, $\mathcal{H}_-$ counts the invariants of the part of the Lorentz and gauge group which transform under C and P transformations. These additional parity transformations can be included by a folding technique [64, 227]. After applying this technique, the Haar measure and character of the negative branch of the Lorentz group are found to be $\widetilde{\text{Lorentz}}_- = \text{Sp}(2)$, while their Haar measure and characters for the $SU(3)_c$ part of the gauge group are $\widetilde{SU(3)}_- = \text{Sp}(2)$. A detailed derivation can be found in Ref. [64].

There is one difficulty for the characters in the odd branch. In the derivation of the Molien-Weyl formula, the fact that the representation matrix of the group element can always be diagonalised on the maximal torus representation. Then, for $g \in G$ it is easy to see, that $\text{Tr}\,(g^p(z_1, \ldots, z_n)) = \chi(z_1^p, \ldots, z_n^p)$. It can be shown, that after the folding procedure that is necessary to compute the characters of the parity-odd branches, the vector representation of matrix for any parity-odd element has two eigenvalues, which are not parameters of the maximal torus representation, but instead just $+1$ and -1 [64]. Then, the identity $\text{Tr}\,(g^p(z_1, \ldots, z_n)) = \chi(z_1^p, \ldots, z_n^p)$ obviously no longer holds true, as for odd powers these last

[19] For a real singlet (pseudo-)scalar a, like that axion we will consider later, the spurion a itself can be used as a building block, as the scalar transforms into itself up to a sign under CP transformations.

[20] We have omitted the $\Delta\mathcal{H}$ terms here. As in Eq. (2.112), these terms should be added to obtain the correct final form of the Hilbert series, as we will discuss later in Sec. 7.3.

two eigenvalues cancel, but for even powers they do not [227]. Instead, the characters for the single particle modules in terms of the characters of the gauge and Lorentz group, appearing in the odd and even powers in the plethystic exponential, should be [105]

$$\text{odd power: } \chi_i^{P^-}(\mathcal{D},\tilde{x})\chi_i^{C^-}(\tilde{z})\,, \quad \text{even power: } \chi_i^{P^+}(\mathcal{D},\bar{x})\chi_i^{C^+}(\bar{z})\,, \tag{2.116}$$

where $\chi_i^{P^\pm}$ is the character corresponding to the Lorentz group, and $\chi_i^{C^\pm}$ is the character of the gauge groups. We have introduced some new notation here, which appears in the folding procedure to obtain the characters of the minus branch of the Lorentz and gauge group. During the folding procedure, some parameters become redundant and the characters depend on fewer parameters, which we denote as $\tilde{x} \equiv x_1$ and $\tilde{z} \equiv (z_{c,1}, z_W)$. This is due to the fact that after diagonalising the matrix representation on the maximal torus (c.f. Eq. (2.91)) of the negative branch of the symmetry group, one of the eigenvalues is ± 1, corresponding to the parity part of the group. Then, the character of the representation will depend on one less parameter with respect to the group without the parity transformation [64]. The corresponding momentum generating functional P_- of the minus branch is defined as

$$P_-(\mathcal{D},\tilde{x}) = \frac{1}{(1-\mathcal{D}x_1)(1-\mathcal{D}x_1^{-1})(1-\mathcal{D}^2)}\,. \tag{2.117}$$

As indicated in Eq. (2.116), the even-power characters are the same as those of the positive branch $\chi^-(\mathcal{D},x,z) = \chi^+(\mathcal{D},\bar{x},\bar{z})$ after setting the parameters which are rendered redundant in the folding procedure are set to unity, i.e. $\bar{x} \equiv (x_1, 1)$ and $\bar{z} \equiv (z_{c,1}, 1, z_W, 1)$. It turns out that for the SM particle content, all of the characters appearing in odd powers of the plethystic exponential vanish because none of the SM particles are transformed into themselves under CP transformations [105]. For a singlet scalar, like the axion we will discuss later, this no longer holds true and the terms in the odd powers of the plethystic exponential are non-vanishing [64, 227]. We will discuss this in Sec. 7.2.1, where we will also show how to encode the shift symmetry of the ALP in its character.

After introducing all the technicalities on how to include CP in the Hilbert series counting, we are now ready to present the Hilbert series for the CP-even and CP-odd operators of the given EFT. They can be obtained as different combinations of the Hilbert series of the plus and minus branch introduced above

$$\mathcal{H}_{\text{even}} = \frac{1}{2}(\mathcal{H}_+ + \mathcal{H}_-)\,, \quad \mathcal{H}_{\text{odd}} = \frac{1}{2}(\mathcal{H}_+ - \mathcal{H}_-)\,, \tag{2.118}$$

where the full Hilbert series, is of course simply given by the part of the Lorentz and gauge group which is left invariant by C and P transformations $\mathcal{H} = \mathcal{H}_{\text{even}} + \mathcal{H}_{\text{odd}} = \mathcal{H}_+$.

CP-violating operators These expressions presented in Eq. (2.118) allow us to obtain the counting of all CP-even and CP-odd operators in the EFT. However, we have found in Secs. 2.1 and 2.2.3 that not all CP-odd operators must necessarily be CP-violating due to flavour transformations which allow to remove CP-odd parameters from the Lagrangian. In the presence of physical Yukawa couplings as they are measured in nature, the SM Lagrangian has an accidental exact flavour group $U(1)^3_{L_i} \times U(1)_B$ corresponding to the lepton family numbers and baryon number, which leaves all couplings in the SM Lagrangian invariant. These rephasings can then be used on the non-renormalisable operators to remove CP-odd parameters from them, if the operator is not invariant under at least one of the $U(1)$ transformations. Therefore, it would be ideal to include this effect in the Hilbert series and count truly CP-violating operators instead of CP-odd operators.

Following Ref. [105], this can be achieved by implementing these rephasing invariants as global symmetries of the fermion fields as is done for the spurions appearing in the flavour invariants and integrating over the additional $U(1)$s to project out the singlets under the rephasings. For EFTs based on the SM particle content, this will simply amount to adding the four $U(1)$ symmetries corresponding to the lepton and baryon numbers $U(1)^3_{L_i} \times U(1)_B$, as was just mentioned.

Later in this thesis, we will also construct effective theories below the electroweak scale, where the heavy particles of the SM, the W, Z, H and top quark are integrated out and $SU(2)$ is spontaneously broken, rendering the left-handed up- and down quarks independent of one another. Then, the exact flavour group in the presence of the fermion masses is increased to $U(1)^3_{e_i} \times U(1)^3_{u_i} \times U(1)^3_{d_i}$, corresponding to lepton and quark family numbers, which are no longer broken by the CKM matrix at the level of the renormalisable Lagrangian. There is no $U(1)$ symmetry in the neutrino sector due to the Majorana nature of the allowed mass term $\bar{\nu}_L \nu_L^c$ at low energies. Therefore, an additional $N_u + N_d + N_e$ of $U(1)$ integrals have to be calculated, one for each active fermion flavour in the effective theory which has not been integrated out yet. Looking at Eq. (2.116), we can immediately realise that the rephasing acts trivially on the negative branch of the gauge group and the additional $U(1)$ integrals only have to be added to the positive branch. Putting everything together, we find that the Hilbert series of the CP-violating operators can be computed by [105]

$$\mathcal{H}_{\mathrm{CPV}} = (U(1)\ \text{inv.}\ \mathcal{H}_+) - \mathcal{H}_- \,. \tag{2.119}$$

2.6 Topological Field Configurations: Instantons

In this section, we will briefly review topical field configurations in QFT and in particular instanton configurations. This section is mainly based on Refs. [37, 229–231], while other good references for the subject are Refs. [142, 232–234]. We will work in Euclidean space throughout this section by performing a Wick rotation $x^0 \to ix^0$.

Most QFT computations in the context of high-energy particle physics are done in perturbation theory by expanding around the saddle-point of the action in the path integral, maximised by the classical field configuration. Here, the action is split into its free, kinetic part S_0 and an interaction part S_{int}, which can be organised in terms of a small coupling constant g, which dictates the validity of perturbation theory. For a real scalar ϕ we can write the path integral of such a scenario as follows

$$\int \mathcal{D}\phi\, e^{-S_0[\phi] - gS_{\text{int}}[\phi]} \tag{2.120}$$

where we have factored the coupling g out of the interacting action.[21] From this action we can compute correlation functions by expanding the exponential of the interacting action. For instance, we can compute the time-ordered vacuum correlator with an insertion of some operator $\mathcal{O}$ as follows

$$\langle 0|T\{\mathcal{O}(x)\}|0\rangle = \int \mathcal{D}\phi\, e^{-S_0[\phi]-gS_{\text{int}}[\phi]}\mathcal{O}(x) = \int \mathcal{D}\phi\, e^{-S_0[\phi]}\left(1 - gS_{\text{int}} + \frac{g^2 S_{\text{int}}^2}{2!} + \mathcal{O}\left(g^3\right)\right)\mathcal{O}(x)\,, \tag{2.121}$$

where subsequently the propagator of the free field in Euclidean space

$$\Delta(x_1 - x_2) = \int \mathcal{D}\phi\, e^{-S_0[\phi]}\phi(x_1)\phi(x_2) \tag{2.122}$$

is used to evaluate the correlator in Eq. (2.121) after all possible contractions of the fields are considered.

There exist however also physical effects, which can never show up in perturbation theory due to their topological nature. As we have already mentioned earlier in Sec. 2.4, one such effect appears in the pure Yang-Mills QCD part of the full SM Lagrangian presented in Eq. (2.1). In Euclidean space, the corresponding action reads

$$S_{\text{YM}} = \int d^4x \left(\frac{1}{4}G^A_{\mu\nu}G^{A,\mu\nu} + i\theta_{\text{QCD}}\frac{g_3^2}{32\pi^2}G^A_{\mu\nu}\tilde{G}^{A,\mu\nu}\right) \tag{2.123}$$

due to the θ term. We are interested in performing semi-classical approximations, because we know how to perform computations with such configurations. Therefore, we are interested in topological configurations of the theory in Eq. (2.123) with finite Euclidean action S_E, which maximises the Euclidean path integral weighted by $\exp\left(-S_E\right)$ [37]. One can rewrite the θ term as the total derivative of the Chern–Simons current j^μ_{CS} [230]

$$G^A_{\mu\nu}\tilde{G}^{A,\mu\nu} = \partial_\mu\epsilon^{\mu\nu\rho\sigma}\left(G^A_\nu G^A_{\rho\sigma} - \frac{g_3}{3}f^{ABC}G^A_\nu G^B_\rho G^C_\sigma\right) \equiv \partial_\mu j^\mu_{\text{CS}}\,, \tag{2.124}$$

which makes it clear that it cannot ever show up in perturbation theory due to Gauss's law assuming that the gauge fields are such that the field strength falls off sufficiently quickly that it goes to zero on the integration boundary, making the action of the theory finite.

The most straightforward way of satisfying this condition is that the gauge fields themselves are zero on the boundary $G^A_\mu|_{\text{bnd}} = 0$. Another way to obtain vanishing field strengths on the boundary is considering gauge transform of the zero gauge field solutions [37]

$$\left(G_\mu|_{\text{bnd}}\right)' = UG_\mu|_{\text{bnd}}U^{-1} + U\partial_\mu U^{-1} = U\partial_\mu U^{-1} \tag{2.125}$$

where $U = \exp\left(i\alpha^A T^A\right)$ is an element of the $SU(3)_c$ gauge group and we have used that the untransformed gauge fields vanish on the boundary. We call field configurations, which

[21] Note, that there could of course be several interactions with different couplings in S_{int} for a real scalar ϕ. We use this simplified situation here where there is a single interaction with the coupling g to exemplify the principles of perturbation theory.

are the gauge transform of a vanishing gauge field, *pure gauge* configurations. There are different choices of gauge transformations in Eq. (2.125) and we should come up with a way of classifying the different solutions in an attempt of finding a structure.

To understand the solutions in Eq. (2.125) better, it is helpful to notice that they are mappings of the boundary of Euclidean space-time, i.e. a three-dimensional hypersphere S^3, into the gauge group [37]. It turns out, that for any simple Lie group G such mappings can be continuously deformed into mappings of an $SU(2)$ subgroup of G [235]. Since, furthermore $SU(2)$ is topologically equivalent to S^3 [230],[22] we are essentially looking for mappings of S^3, as the boundary of Euclidean space-time, onto S^3, the gauge group space. These mappings of S^3 onto itself can be classified in an intuitive way by counting how many times one sphere covers the other sphere, i.e. how many times one has to wind around one sphere to wind around the other sphere once. Mathematically, this is expressed in terms of homotopy groups $\pi_n(G)$, which classify the mappings of an n-sphere S^n onto a group G. The relevant group for a 4-dimensional Euclidean space-time is the third homotopy group of S^3 denoted by

$$\pi_3(S^3) = \mathbb{Z}\,. \tag{2.126}$$

We call topological field configurations following this mapping *instantons*.[23] As a consequence we can put the topological solutions into equivalence classes labelled by a single $Q \in \mathbb{Z}$. We will refer to this number as the winding number or topological charge of the configuration and it can be computed directly from the gauge configuration as follows [37]

$$\frac{g_3^2}{32\pi^2} \int d^4x\, G^A_{\mu\nu} \tilde{G}^{A,\mu\nu}(x) = Q \in \mathbb{Z}\,. \tag{2.127}$$

This has important consequences for the vacuum structure of the theory. We can identify a vacuum state, where the field strength tensor $G^a_{\mu\nu}$ vanishes, with a pure gauge configuration with winding number n and the corresponding state labelled by $|n\rangle$ [150]. As discussed before, any further gauge transformation can change the winding number of the vacuum. Hence, the true vacuum should be the super position of all the topological configurations. We define the combination [236]

$$|\theta\rangle = \sum_{n=-\infty}^{n=\infty} e^{in\theta}|n\rangle\,, \tag{2.128}$$

which we call the θ vacuum. Here, $\theta \in [0, 2\pi)$ is the vacuum angle, which as we will see now can be identified with the θ term in the action Eq. (2.123).

We will now compute the dependence of the vacuum energy on θ, which will allow us to understand how to resolve the strong CP problem. To perform these computations we will

[22] This can be appreciated by defining an $SU(2)$ matrix $M = A\mathbb{1} + i\mathbf{B}\sigma$, with σ the vector of Pauli matrices and A and $\mathbf{B}$ are 4 real parameters. Imposing that $M^\dagger M = \mathbb{1}$ and $\det M = 1$, yields the condition $A^2 + \mathbf{B}^2 = 1$, which describes a 3-dimensional sphere [230].

[23] We can understand other topological solutions of QFT in a similar way. Monopoles can be understood by mappings of the two-dimensional spatial boundary into the gauge group, vortices as a mapping of a one-dimensional boundary into the gauge group and domain walls or kinks, with a co-dimension of one. They can all be classified by the respective homotopy group [234].

work with a specific gauge configuration, featuring all the properties discussed above – the Belavin–Polyakov–Schwarz–Tyupkin (BPST) instanton [237]. This instanton configuration has winding number $Q = \pm 1$ and can be understood as the field configuration which interpolates between a vacuum with winding number n and one with winding number $n+1$. Working in the regular Landau gauge, the gauge field of the BPST instanton solution based on an $SU(2)$ gauge group has the following form [237]

$$G_\mu(x) = 2\,\eta_{a\mu\nu} t^a \frac{(x-x_0)_\nu}{(x-x_0)^2+\rho^2}\,, \quad \eta_{a\mu\nu} = \begin{cases} \epsilon_{a\mu\nu}, & \mu,\nu \in \{1,2,3\} \\ -\delta_{a\nu}, & \mu = 0 \\ +\delta_{a\mu}, & \nu = 0 \\ 0, & \mu = \nu = 0 \end{cases} . \tag{2.129}$$

Hence, $a = 1, 2, 3$, t^a are the generators of $SU(2)$ and $\eta_{a\mu\nu}$ are the 't Hooft η symbols [143]. To obtain the instanton solutions for an $SU(N)$ gauge theory, the $SU(2)$ solution can be embedded into the $SU(N)$ group. In the following, we will work with the minimal embedding, where the $SU(2)$ instanton solution in embedded into the upper left corner of the $SU(N)$ generators of the fundamental representation. With the $Q = 1$ instanton solution also comes an anti-instanton solution with opposite topological charge $Q = -1$. The corresponding gauge field has the same functional form as the instanton solution in Eq. (2.129), where the 't Hooft symbols denoted by $\bar{\eta}_{a\mu\nu}$ for the anti-instantons are modified as $\delta_{a\mu}, \delta_{a\nu} \to -\delta_{a\mu}, \delta_{a\nu}$ with respect to the original η.

The BPST instanton solution in Eq. (2.129) is parameterised by its location given by the Euclidean four-vector x_0^μ and its size ρ, as well as the 3 gauge parameters α^a corresponding to gauge transformations of the vector potential in Eq. (2.129). Those parameters are referred to as the collective coordinates of the instanton solution. Later, we are interested in QCD instantons based on the $SU(3)_c$ group. In the embedding of the $SU(2)$ instanton solution into an $SU(N)$ group, there is the freedom in choosing an $SU(2)$ subgroup of $SU(N)$, into which the solution is embedded [230]. We will work with the minimal embedding, which puts the $SU(2)$ instanton solution in the upper left corner of the $SU(N)$ solution [231]

$$G_\mu^{SU(N)} = \begin{pmatrix} G_\mu^{SU(2)} & 0 \\ 0 & 0 \end{pmatrix}, \tag{2.130}$$

corresponding to the following choice of generators of the fundamental representation of $SU(N)$ [230]

$$T^1 = \frac{1}{2}\left(\begin{array}{cc|c} 0 & 1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 0 \end{array}\right), \quad T^2 = \frac{1}{2}\left(\begin{array}{cc|c} 0 & -i & 0 \\ i & 0 & 0 \\ \hline 0 & 0 & 0 \end{array}\right), \quad T^3 = \frac{1}{2}\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 0 \end{array}\right), \tag{2.131}$$

where the zeros outside of the matrix in the upper left corner fill up the remaining entries of the $N \times N$ matrices. For instance, for $SU(3)$, which will use in the computations below, the generators are simply the first three Gell-Mann matrices $T^a = 1/2\,\lambda^a$, $a = 1, 2, 3$. After choosing this embedding, there is still the freedom to perform general $SU(N)$ gauge transformations on the solution, where only the subgroup of $SU(N)$ transformations generates a new solution, which leaves the embedding invariant. Performing an $SU(N)$ gauge transformation U on Eq. (2.130),

$$G_\mu^{SU(N)} = U \begin{pmatrix} G_\mu^{SU(2)} & 0 \\ 0 & 0 \end{pmatrix} U^\dagger \,, \tag{2.132}$$

it is straightforward to see, that there is a subgroup $U \in SU(N-2) \times U(1)$ of gauge transformations acting only on the zeros in Eq. (2.130), that leaves the solution invariant. Hence, in total, for an $SU(2)$ instanton solution, we have 5 parameters from the translations (changing the instanton centre x_0^μ) and dilatations (changing the instanton size ρ) as well as 3 parameters from the group transformations, that yield new instanton solutions. After embedding the $SU(2)$ solution into the $SU(N)$ group, there are an additional $N^2-1-((N-2)^2-1)-1 = 4N-5$ parameters describing the freedom of gauge transformations after the embedding [231].

Later while performing computations, we will mostly work with the field strength, which for the instanton solution in Eq. (2.129) reads

$$G_{\mu\nu} = -4\,\eta_{a\mu\nu} t^a \frac{\rho^2}{((x-x_0)^2 + \rho^2)^2} \,. \tag{2.133}$$

An important property of the (anti-)instanton configurations is that their field strength is (anti-)self-dual

$$G_{\mu\nu} = \pm \tilde{G}_{\mu\nu} \,, \tag{2.134}$$

where the plus is for the instanton solution and the minus sign appears for the anti-instanton solution. This is easy to see by requiring that the Euclidean action [230]

$$\int d^4x\, \frac{1}{4} G^A_{\mu\nu} G^{A,\mu\nu} = \int d^4x\, \frac{1}{4} G^A_{\mu\nu} \tilde{G}^{A,\mu\nu} + \frac{1}{8}\left(G^A_{\mu\nu} - \tilde{G}^A_{\mu\nu}\right)^2 = Q\frac{8\pi^2}{g_3^2} + \frac{1}{8}\int d^4x\, \left(G^A_{\mu\nu} - \tilde{G}^A_{\mu\nu}\right)^2 \,, \tag{2.135}$$

be minimal. Looking at the last equality this is clearly the case when Eq. (2.134) is satisfied. Note, that we have used the definition of the topological charge Q in the second step. The (anti-)self-duality property of the instanton solution also ensures that the classical equation of motion is fulfilled [230]

$$D^\mu G^A_{\mu\nu} = D^\mu \tilde{G}^A_{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\rho\sigma} D^\mu G^{A,\rho\sigma} = \frac{1}{6}\epsilon_{\mu\nu\rho\sigma}\left(D^\mu G^{A,\rho\sigma} + D^\rho G^{A,\sigma\mu} + D^\sigma G^{A,\mu\rho}\right) = 0 \,, \tag{2.136}$$

due to the Bianchi identity used in the last step. Plugging a BPST instanton of topological charge Q[24] in the Yang-Mills action yields the following finite action

$$S_{\text{BPST},Q} = \frac{8\pi^2}{g_3^2}|Q| + iQ\theta_{\text{QCD}}\,. \tag{2.137}$$

Two comments are in order. Firstly, the expression in Eq. (2.137) clarifies why we only considered the $Q = \pm 1$ instanton solutions, as they dominate the path integral proportional to $\exp(-S_{\text{BPST}})$. Furthermore, this equation also makes it clear that the instanton is a non-perturbative effect, because its action is proportional to inverse powers of the gauge coupling g_3, which could never be generated in perturbation theory. Note however, that the gauge coupling still needs to remain in the perturbative regime for the semi-classical approximation we made earlier still to hold true. Indeed, the semi-classical approximation works best when the Euclidean action in Eq. (2.137) is large, i.e. when g_3 is small [142]. That is why instantons cannot be used reliably in QCD at low energies, opposed to the early hopes of understanding non-perturbative QCD analytically by use of them. Later this was referred to as an "IR embarrassment" by Coleman [37]. This is alleviated in computations of QCD at finite temperature, where the temperature acts as a lower IR cut-off in the integral over the instanton size [238].

After the discussion of all the properties of the BPST instanton, we are finally ready to compute the vacuum energy density $E(\theta)$ of the theory, which in the limit of large 4-volumes V_4 is related to the Euclidean generating functional $Z[\theta]$ as follows [150]

$$Z[\theta] = \lim_{V_4\to\infty} e^{-E(\theta)V_4}\,, \tag{2.138}$$

where the generating functional of the BPST 1-instanton solution is

$$Z[\theta] = \int \mathcal{D}G_\mu \exp\left(\int d^4x \left(-\frac{1}{4}GG + i\theta\frac{g_3^2}{32\pi^2}G\tilde{G}\right)\right) \sim e^{i\theta}e^{-\frac{8\pi^2}{g_3^2}}\,, \tag{2.139}$$

where we have used the semi-classical approximation in the last step and ignored all quantum fluctuations around it. Adding the generating functional of the anti-instanton solution to this and summing over all possible instanton configurations with topological charge Q in the dilute gas limit, where the instantons and anti-instantons are well-separated, yields [37]

$$E(\theta) = -2Ke^{-\frac{8\pi^2}{g_3^2}}\cos\theta\,, \tag{2.140}$$

where K is a constant generated by the integration over the instanton zero modes.

We have discussed in Sec. 2.4, that we can relax the vacuum angle θ to zero by making it dynamical. Indeed, the potential in Eq. (2.140) generated for such a dynamical θ-angle would be minimised at zero (assuming a solution for the cosmological constant problem), solving the

[24] This solution can be obtained by taking the gauge transformation U that generates the 1-instanton pure gauge field by $G_\mu = U\partial U^{-1}$ and taking it to the Qth power [230]. The gauge transformation obtained that way will generate a charge-Q instanton gauge configuration with the same "pure gauge" mapping.

strong CP problem. We already discussed earlier that instantons are not reliable in the regime where QCD confines. Hence, we cannot use the computations presented here to compute the potential of the QCD axion. Indeed, as discussed in Sec. 2.4.1 χPT should be used to compute the QCD axion potential instead. There could however be configurations in the UV, which change the gauge coupling of QCD in a such a way, that instanton effects become important again while still being reliable [239]. In such cases, the instanton configurations can change the potential of the QCD axion presented in Eq. (2.53), increasing the mass of the axion for UV contributions which are aligned with the QCD potential or even destroy the solution to the strong CP problem if they are misaligned.

Misaligned contributions are generated in the presence of new sources of CP violation in the UV and we will study them in the SMEFT framework in Chap. 8. This requires us to discuss the presence of fermions charged under the gauge groups responsible for the instantons. The Euclidean action of the massless quarks of the SM reads

$$S_\psi = \int d^4x\, \bar{\psi}_f\big(-i\not{D}\big)\psi_f\,, \tag{2.141}$$

whose EOM is the Dirac equation. To study the influence of the instantons on the massless quarks, we will expand the fermions in eigenmodes of the Dirac operator

$$i\not{D}\psi^{(n)} = \lambda_n \psi^{(n)}\,, \tag{2.142}$$

where the λ_n are the real eigenvalues of the Dirac operator and we have expanded $\psi = \sum_{i=0}^{\infty}\psi^{(n)}\xi_\psi^{(n)}$ with $\psi^{(n)}$ the wave function of the nth eigenmode and $\xi_\psi^{(n)}$ are Grassmannian vectors. Then, for the zeroth eigenmode, also called zero mode for short, we have

$$i\not{D}\psi^{(0)} = i\left(\not{\partial} + ig_3\not{G}\right)\psi^{(0)} = 0\,. \tag{2.143}$$

Plugging in the explicit $Q = 1$ BPST solution for the vector gauge field in Eq. (2.129), we find that the zero mode of the quark fields also has a special functional form in the instanton background. In regular Landau gauge, the zero modes read as follows [230, 232]

$$\psi^{(0)}(x) = \begin{pmatrix}\chi_L\\ \chi_R\end{pmatrix} = \frac{1}{\pi}\frac{\rho}{\left[(x-x_0)^2+\rho^2\right]^{3/2}}\begin{pmatrix}0\\ \varphi\end{pmatrix}\,,\qquad \varphi_{\alpha k} = \epsilon^{\alpha k}\,, \tag{2.144}$$

where $\alpha = 1,2$ and $k = 1,2$ are the spin and colour indices, respectively. They are entangled by the Levi–Civita symbol as was also the case for the gauge field solution in the instanton background. The zero modes are normalised to unity $\int d^4x\, \psi^{(0)\dagger}\psi^{(0)} = 1$. Note, that only the right-handed chiral fermions $\chi_L^\dagger, \chi_R$ receive a non-vanishing contribution in the instanton background, while only the left-handed Weyl fermions receive a contribution in the anti-instanton background.

To compute the additional contributions to the vacuum energy or the potential of the axion for a dynamical vacuum angle in Chap. 8, we have to compute correlators with different operator insertions in the instanton background in Euclidean space, which we will do directly from the path integral. We will follow the seminal paper by 't Hooft [143] expressed in the notation of Ref. [240]. Then, a correlation function with an insertion of an operator $\mathcal{O}$ can be computed directly from the path integral by integrating over all gauge fields A_μ, ghost fields η, scalars ϕ and fermions ψ of the SM as follows

$$\langle 0|\mathcal{O}|0\rangle\big|_{\text{1-inst.}} = \frac{\int \mathcal{D}A_\mu \mathcal{D}\eta\mathcal{D}\bar{\eta}\mathcal{D}\phi\mathcal{D}\phi^\dagger\mathcal{D}\psi\mathcal{D}\bar{\psi}\, e^{-S_E}\mathcal{O}\big|_{\text{1-inst.}}}{\int \mathcal{D}A_\mu \mathcal{D}\eta\mathcal{D}\bar{\eta}\mathcal{D}\phi\mathcal{D}\phi^\dagger\mathcal{D}\psi\mathcal{D}\bar{\psi}\, e^{-S_E}\big|_{A_\mu^{\text{cl}}=0}}\,. \tag{2.145}$$

To simplify the computation of this correlator, we can make several simplifications thanks to the semi-classical instanton background we work in. First, all fields not taking part in the instanton dynamics, i.e. those which are not charged under $SU(3)_c$, can be treated as in ordinary perturbation theory as laid out at the beginning of this section by expanding the interacting action in its small coupling and using the definition of the propagator to contract all fields.

Second, all other fields which are involved in the instanton dynamics are split into their zero modes and non-zero modes as explained throughout this section. Splitting, $G = G^{(0)} + G'$ for the gluon fields and $\psi = \psi^{(0)} + \psi'$, where the fields with a superscript (0) are the zero modes of the fields, which can be found in Eqs. (2.129) and (2.144) and the primed fields are the non-zero modes. We then expand the action to second order in the fields around their semi-classical background

$$S_E = S_0(\rho) + \int d^4x \sum_i \Phi_i'^\dagger M_{\Phi_i'} \Phi_i'\,, \tag{2.146}$$

where Φ' collects all the non-zero modes of the gluon fields, ghosts and quarks. S_0 contains only zero modes of the fields partaking in the instanton dynamics, however it can still contain non-zero modes of other fields not charged under the group, like the Higgs or lepton interactions.

We will start by performing the integration over the non-zero modes of the fermions. We want to emphasise again, that we only keep the non-zero modes up to quadratic order here but for instance ignore the Yukawa interactions between non-zero modes of quarks with the Higgs, which we simply expand to zeroth order in the small perturbative coupling. Splitting the fermions into zero modes and non-zero modes, changes the path integration measure as follows [240]

$$\mathcal{D}\psi\mathcal{D}\bar{\psi} = \prod_f \|\psi_f^{(0)}\|^{-1} d\xi_f^{(0)} \|\bar{\psi}_f^{(0)}\|^{-1} d\bar{\xi}_f^{(0)} \mathcal{D}\psi'\mathcal{D}\bar{\psi}'\,. \tag{2.147}$$

Here, $\psi_f^{(0)}$ are the zero mode wave function from Eq. (2.144), where f collects all internal indices like flavour indices or gauge indices of other groups not partaking in the instanton dynamics, and $d\xi_f^{(0)}, d\bar{\xi}_f^{(0)}$ are Grassmann integration measures. The action of the zero modes simply vanishes by definition of the zero modes. The remaining integral over the non-zero modes is Gaussian and simply yields a determinant, which was first computed in Ref. [143]

and contributes to the instanton density $d_N(\rho)$ to be defined below. In total, we find

$$\int \mathcal{D}\psi\mathcal{D}\bar{\psi} \to e^{-\frac{2}{3}N_f \log(\rho\mu)+2N_f\alpha(1/2)} \int \prod_{f=1}^{N_f} \left(\rho d\xi_f^{(0)} d\bar{\xi}_f^{(0)}\right), \tag{2.148}$$

where α is a function defined in Ref. [143], that we will numerically evaluate below, when we give the final result for the instanton density. Note, that $\frac{2}{3}N_f$ is the fermion contribution to the 1-loop QCD β-function.

Next, we perform the integration over the quadratic action of the non-zero modes of the bosonic fields, i.e. in our case the gluon fields and their ghosts. This will lead to a determinant of the bosonic matrices $M_{\Phi_i'}$ that has to be computed. We will just give the result here and refer to Ref. [143] for the details. The action of the zero modes will simply reduce to that of Eq. (2.137) for the bosonic contributions, where replacing the functional integration over the zero modes with the collective coordinates gives rise to a Jacobian. In total we find

$$\int \mathcal{D}A_\mu \mathcal{D}\eta\mathcal{D}\bar{\eta} \to e^{-i\theta_{\text{QCD}}} \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho), \tag{2.149}$$

where $d_N(\rho)$ is the instanton density which appears after integrating over the non-zero modes of the gauge fields and parameterising the zero modes in terms of their collective coordinates. We find for the instanton density

$$d_N(\rho) = C[N] \left(\frac{8\pi^2}{g^2}\right)^{2N} e^{-8\pi^2/g^2(1/\rho)}, \tag{2.150}$$

where the factor $g^2(1/\rho)$ in the exponential is the running gauge coupling induced by the integration over the non-zero modes as we saw more or less explicitly for the fermions in Eq. (2.148). Including both the contributions of the gauge fields and fermions, the full running is given by

$$\frac{8\pi^2}{g^2(1/\rho)} = \frac{8\pi^2}{g_0^2(\mu)} - b_0 \log(\rho\mu), \quad b_0 = \frac{11}{3}N - \frac{2}{3}N_f. \tag{2.151}$$

The prefactor $\left(\frac{8\pi^2}{g^2}\right)^{2N}$ is due to the Jacobian arising when the gauge field zero modes are parameterised in terms of the collective coordinates. Here, the gauge coupling should be understood as the bare coupling and any running effects are effectively of two-loop order in the computation. Finally, the first term also comes from the integration over the non-zero modes on top of the beta function giving the running coupling. The factor $C[N]$ reads as follows [143, 240–242]

$$C[N] = \frac{C_1\, e^{-C_2 N}}{(N-1)!(N-2)!}\, e^{0.292N_f}, \tag{2.152}$$

where $C_1 \approx 0.466$, $C_2 \approx 1.678$ and the integration over the fermion non-zero modes yields the factor $e^{0.292N_f}$. Note, that C_2 and the exponential factor are scheme-dependent [143]. Here, we have shown them in the Pauli–Villars regularisation scheme.

Part I

CP Violation in the Presence of Massive Neutrinos

3

The Flavour Invariants of the Standard Model Extended with Sterile Neutrinos

3.1 Introduction

In Sec. 2.3, we have introduced different ways of generating the neutrino masses observed in Nature. In both the νSM and the type-I seesaw model right-handed neutrinos are introduced, which generate the neutrino masses either by their direct small couplings to the SM degrees of freedom in the νSM, or via the seesaw mechanism if their Majorana mass is large. Either way, by adding new flavourful couplings to the theory, new perturbative sources of CP violation are added to the Lagrangian. Since, the status of CP violation in the lepton sector is not yet fully determined, it is an interesting task to classify the new sources of CP violation by using flavour invariants, as was introduced in Sec. 2.1 for the CKM-phase of the SM.

To this end, we will use the Hilbert series and related tools from invariant theory introduced in Sec. 2.5.1 to count the number of generating invariants and the relations among them. The set of generating invariants will in principle allow us to express any observable in the theory as a function of the invariants. This is particularly interesting for CP-odd observables as they could reveal the intricate structure of flavourful CP violation in the theory through the invariants. For instance, demanding that the flavour-invariant CP-odd structures are generated in perturbation theory, allows us to make statements about the order in the couplings at which certain phases can appear in observables. As we will see in the following sections, the invariants will also allow us to easily differentiate between the Dirac and Majorana nature of the mass term and allow us to make statements about the theory in the seesaw limit. Here, we can show that while all parameters present in the effective theory of the νSM appear suppressed with only one or two powers of the heavy Majorana mass, they can only appear in a flavour-invariant way with a suppression of two and four powers of the Majorana mass.

Invariants have been used both in UV complete theories [218, 220, 243–255] and EFTs to characterise the parameters of the theory with respect to CP [103, 104, 256–258]. Some problems which are closely related to the analysis presented here have been previously investigated in the literature. In particular, the νSM with only two generations of charged leptons

	$SU(3)_L \times U(1)_L$	$SU(3)_e \times U(1)_e$	$SU(3)_N \times U(1)_N$	$U(1)_{L+e+N}$
Y_e	$\mathbf{3}_{+1}$	$\bar{\mathbf{3}}_{-1}$	$\mathbf{1}_0$	0
Y_N	$\mathbf{3}_{+1}$	$\mathbf{1}_0$	$\bar{\mathbf{3}}_{-1}$	0
M_N	$\mathbf{1}_0$	$\mathbf{1}_0$	$(\bar{\mathbf{3}} \otimes_s \bar{\mathbf{3}})_{-2}$	-2
$X_e = Y_e Y_e^\dagger$	$(\mathbf{3} \otimes \bar{\mathbf{3}})_0$	$\mathbf{1}_0$	$\mathbf{1}_0$	0
$X_N = Y_N Y_N^\dagger$	$(\mathbf{3} \otimes \bar{\mathbf{3}})_0$	$\mathbf{1}_0$	$\mathbf{1}_0$	0
$X_M = M_N M_N^*$	$\mathbf{1}_0$	$\mathbf{1}_0$	$(\bar{\mathbf{3}} \otimes \mathbf{3})_0$	0

Table 3.1: The flavour transformation properties of the relevant Yukawa matrices and Majorana mass matrix treated as spurions. The subscripts of the $SU(3)$ representations denote the charge under the $U(1)$ part of the flavour symmetry group. Furthermore, $\otimes_s$ denotes the symmetric tensor product of the simple representations. The charges of all spurions under Abelian lepton number transformations are indicated in the last column. We also show the transformation properties of X_e, X_N and X_M, which will be used in following sections.

and neutrinos has been studied in Ref. [218] and the case of adding two generations of right-handed sterile neutrinos to the SM has been treated in Ref. [252]. There, the authors also use the flavour invariants to formulate the necessary and sufficient conditions for CP violation (CPV) in the model. The Hilbert series of the νSM with three generations has previously been reported on in Refs. [224, 257]. Our main result will be the construction of the generating set of flavour invariants of the νSM[1], which allows us, for instance, to capture the sufficient conditions for CP conservation (CPC) in the theory. Unlike in the SM, where the generating set of invariants only contains 14 invariants (c.f. Sec. 2.5.1), the number of generating jumps to 459 invariants for three generations of sterile neutrinos, even though the number of flavourful physical parameters only approximately doubles. This reveals the rich algebraic structure of the flavourful sector of the νSM, captured by these invariants. As a consequence of the complicated algebraic structure of the non-complete intersection ring, there are non-trivial cancellations in the plethystic logarithm which is often used to count invariants given a set of building blocks and their transformation properties. Hence, one should take care when solely relying on these tools from invariant theory to build a complete basis of flavour invariants.

3.2 Building an Invariant Basis for the νSM

We have introduced the Lagrangian of the νSM, the SM extended with three generations[2] of sterile neutrinos, whose flavourful structure we will study here, in Eq. (2.43). We will repeat

[1] Note, that the νSM has the same structure as the type-I seesaw model, where the only difference is the value of the parameters. Since we will keep all parameters generic here, we will refer to the theory as the νSM here for brevity.

[2] In principle 2 generations of sterile neutrinos are enough to generate the observed neutrino masses at low energies [259]. As mentioned before this case has been treated in Ref. [252].

it here for convenience

$$\mathcal{L}_{\nu\text{SM}} = \mathcal{L}_{\text{SM}} + \bar{N} i \not{\partial} N - \left(\bar{L} Y_N \tilde{H} N + \frac{1}{2} \bar{N}^c M_N N + \text{h.c.} \right) . \tag{3.1}$$

The kinetic term of the νSM Lagrangian in Eq. (3.1) is invariant under $U(3)$ flavour transformation, one for each of the fermion flavour multiplets. In the following, we assume that this flavour symmetry is only softly broken by the Yukawa couplings and Majorana mass term. Then, we can promote all flavourful couplings to spurions under this symmetry, formally reinstating the symmetry in the Lagrangian. The spurious transformations of all flavourful parameters in the theory can be found in Tab. 3.1. From the tranformations of the Majorana mass matrix M_N one can immediately read off that its presence breaks lepton number, as universal rephasings of N are broken by the Majorana character of the mass term. As a consequence, there will be additional physical Majorana-type phases in the spectrum of the theory.

Whenever needed, we will work in an explicit parameterisation of the flavourful matrices. One minimal parameterisation which only contains as many parameters as there are physical parameters in the theory is given by[3]

$$Y_e = \text{diag}\,(y_e, y_\mu, y_\tau) \ , \quad Y_N = V \cdot \text{diag}\,(y_1, y_2, y_3) \cdot W^\dagger, \quad M_N = \text{diag}\,(m_1, m_2, m_3) \ , \tag{3.2}$$

where

$$V = U(\theta_{12}, \theta_{13}, \theta_{23}, \delta) \cdot \text{diag}\left(1, e^{i\phi_1}, e^{i\phi_2}\right), \ W = \text{diag}\left(1, e^{i\phi'_1}, e^{i\phi'_2}\right) \cdot U(\theta'_{12}, \theta'_{13}, \theta'_{23}, \delta') \ , \tag{3.3}$$

and $U(\theta_{12}, \theta_{13}, \theta_{23}, \delta)$ has the same form as the CKM matrix defined in Eq. (2.3) with a phase $\delta \in [0, 2\pi)$ and three mixing angles $\theta_{ij} \in [0, \pi/2]$. $\phi_{1,2} \in [0, 2\pi)$ and $\phi'_{1,2} \in [0, \pi)$ are additional phases. This parameterisation correctly captures the 9 mass parameters, 6 mixing angles and 6 phases of the theory. A detailed counting from a symmetry perspective can be found in Tab. 3.2.

By setting the Majorana mass term M_N to zero, we can recover Dirac masses for the neutrinos, as discussed in Sec. 2.3. Then, the Yukawa sector of the theory has the same structure as that of the SM quark sector and the mixing matrix W and the phases $\phi_{1,2}$ become unphysical. In this case the PMNS matrix arises in the same way as the CKM matrix in the quark sector of the SM.

Another interesting limit is the seesaw limit, where the Majorana masses are large and hence the Majorana component of the fermions can be integrated out, generating light neutrino masses for the left-handed SM neutrinos, as discussed in Sec. 2.3. Due to the existence of the Majorana mass term, some rephasings are not allowed, and the two additional *Majorana* phases become physical.

[3] A detailed discussion about this parameterisation can be found in Ref. [218] and App. 3.A. There, new parameterisations, which are more convenient for the study of the algebraic properties of polynomial rings, are introduced.

	Real Parameters	Imaginary Parameters	Total
Y_e, Y_N, M_N	$2 \times 9 + 6$	$2 \times 9 + 3$	45
U_L, U_e, U_N	3×3	$3 \times 6 - 3$	24
Difference	15	6	21

Table 3.2: Number of physical parameters in the generic vevs of the flavour spurions Y_e, Y_N, M_N of the νSM presented in Tab. 3.1. Note here, that $U_L, U_e, U_N \in SU(3)$ because the lepton numbers are broken by the presence of the vev of M_N as discussed in the main text and cannot be used to remove imaginary parameters, hence the '-3' in the second column.

3.2.1 Hilbert Series of the νSM

Before we start with the construction of the *generating* and *primary* set of invariants, we will first perform a counting of them using the Hilbert series and plethystic logarithm to set our expectations. To this end, we use the Molien–Weyl formula introduced in Eq. (2.90) to calculate the Hilbert series for the flavour invariants of the νSM with the spurion content Y_e, Y_N and M_N.[4] For the evaluation of the Molien–Weyl formula, we need the characters of the flavourful building blocks appearing in the invariants, constructed from the fundamental and anti-fundamental representations, and the Haar measure of $U(3)$. We have computed the characters in Eqs. (2.92) and (2.93) and the Haar measure can be found in Ref. [64]. They read

$$\begin{aligned} \chi^{\mathbf{3}}_{U(3)} &= z_1 + z_2 + z_3 \,, \\ \chi^{\bar{\mathbf{3}}}_{U(3)} &= z_1^{-1} + z_2^{-1} + z_3^{-1} \,, \\ d\mu_{U(3)} &= \frac{1}{6!} \left(\prod_{i=1}^{3} \frac{dz_i}{2\pi i z_i} \right) \left(- \frac{(z_2 - z_1)^2 (z_3 - z_1)^2 (z_3 - z_2)^2}{z_1^2 z_2^2 z_3^2} \right) . \end{aligned} \tag{3.4}$$

From these, the characters for the representations of the flavourful Lagrangian parameters of the νSM can be constructed following Tab. 3.1. For instance, the character for Y_N is given by

$$\chi_{Y_N} = \chi^{\mathbf{3}}_{U(3)_L}(z_1, z_2, z_3) \chi^{\bar{\mathbf{3}}}_{U(3)_N}(z_4, z_5, z_6) = (z_1 + z_2 + z_3) \left(z_4^{-1} + z_5^{-1} + z_6^{-1} \right) , \tag{3.5}$$

and the characters for all other spurions can be obtained in the same way. Then, we compute the Hilbert series evaluating the expression for the Molien–Weyl formula in Eq. (2.90), where we first use the same grading for all spurions to obtain the ungraded Hilbert series. The calculation amounts to solving the complex integral over the six variables $z_1, \ldots, z_6$ over the contour $|z_i| = 1$, which can be done by calculating the residues. The same calculation has been presented before and we refer to Refs. [224, 257] for the details. We split the Hilbert series into its numerator and denominator to study their form separately. The numerator of

[4] To make M_N dimensionless like the other flavourful couplings in a theory, we divide it by the only other mass scale in the problem, the Higgs vev v. Only then, invariants with a different number of insertions of M_N can be compared.

the Hilbert series reads

$$\begin{aligned}
&\mathcal{N}(q) = \\
&1 + q^4 + 5q^6 + 9q^8 + 22q^{10} + 61q^{12} + 126q^{14} + 273q^{16} + 552q^{18} + 1038q^{20} \\
&+ 1880q^{22} + 3293q^{24} + 5441q^{26} + 8712q^{28} + 13417q^{30} + 19867q^{32} + 28414q^{34} + 39351q^{36} \\
&+ 52604q^{38} + 68220q^{40} + 85783q^{42} + 104588q^{44} + 123852q^{46} + 142559q^{48} + 159328q^{50} \\
&+ 173201q^{52} + 183138q^{54} + 188232q^{56} + 188232q^{58} + 183138q^{60} + 173201q^{62} + 159328q^{64} \\
&+ 142559q^{66} + 123852q^{68} + 104588q^{70} + 85783q^{72} + 68220q^{74} + 52604q^{76} + 39351q^{78} \\
&+ 28414q^{80} + 19867q^{82} + 13417q^{84} + 8712q^{86} + 5441q^{88} + 3293q^{90} + 1880q^{92} + 1038q^{94} \\
&+ 552q^{96} + 273q^{98} + 126q^{100} + 61q^{102} + 22q^{104} + 9q^{106} + 5q^{108} + q^{110} + q^{114},
\end{aligned} \tag{3.6}$$

which is of palindromic form.[5] The denominator is

$$\mathcal{D}(q) = \left(1-q^2\right)^3 \left(1-q^4\right)^4 \left(1-q^6\right)^4 \left(1-q^8\right)^2 \left(1-q^{10}\right)^2 \left(1-q^{12}\right)^3 \left(1-q^{14}\right)^2 \left(1-q^{16}\right) \tag{3.7}$$

As expected, the powers of the factors in the denominator add up to 21, the number of physical parameters in the νSM which is also the cardinality of the *primary* set. Our result of the ungraded Hilbert series is consistent with those found in Refs. [224, 257]. We have furthermore calculated the multi-graded Hilbert series with different parameters $\{e, m, n\}$ counting the degrees of the couplings $\{Y_e, M_N, Y_N\}$, which we only show in App. 3.B due to its length. To obtain these results a `Mathematica` code that can efficiently calculate the Hilbert series was developed, which we will also use later in Chap. 7 to compute the Hilbert series for operator bases in ALP EFTs. The code will shortly be published as a `Mathematica` package under the name `CHINCHILLA` [260].

Furthermore, we can compute the ungraded plethystic logarithm by plugging the ungraded Hilbert series in Eq. (2.94). We find

$$\begin{aligned}
\mathrm{PL}[\mathcal{H}(q)] =& 3q^2 + 5q^4 + 9q^6 + 10q^8 + 19q^{10} + 40q^{12} + 66q^{14} + 92q^{16} + 70q^{18} - 124q^{20} \\
&- 703q^{22} - 2039q^{24} - 4391q^{26} - 7472q^{28} - 8522q^{30} + 590q^{32} + O(q^{34}) .
\end{aligned} \tag{3.8}$$

The plethystic logarithm is a non-terminating series and we only show terms up to order 32. At higher orders, both positive and negative terms will appear repeatedly in an infinite series, which implies that the flavour invariants of the νSM form a *non-complete intersection* ring.

In the usual interpretation of the plethystic logarithm, the leading positive terms in

[5] Note that both in the numerator in Eq. (3.6) and in the denominator in Eq. (3.7) a term $(1+q^2)$ can be factorised, which would slightly simplify the Hilbert series. However, if this factor were to be simplified, the Hilbert series would take a rational form with a numerator featuring some negative terms, in contradiction with the positivity requirement announced earlier for the ungraded Hilbert series. This hints at a more general class of modifications that can be applied to the Hilbert series. Indeed, both numerator and denominator can always be multiplied by a factor $(1+q^k)^m$, if there exists a factor $(1-q^k)^n$ (where $m \leq n$) in the denominator. This multiplication removes a factor of $(1-q^k)^m$ from the denominator while introducing a new factor of $(1-q^{2k})^m$. The total number of factors in the denominator does not change, and the numerator keeps its palindromic form with positive terms. This freedom indicates that there is ambiguity in determining the form of the Hilbert series if there is no further requirement of the Hilbert series. Accordingly, the interpretation of the Hilbert series changes, as now a primary invariant and some of the syzygies are shifted to different degrees in the spurions.

Eq. (3.8) suggest that there exists a total of 314 generating invariants. However, during the explicit construction of the invariants later, we will find that this number is incorrect. While constructing the invariants, we find discrepancies between the number of invariants suggested by the plethystic logarithm and the number of independent irremovable generating invariants, first at order 16, where the counting of generating invariants exceeds the 92 invariants suggested by the plethystic logarithm. This is due to the non-complete intersection nature of the ring, resulting in non-trivial cancellations between the number of generating invariants and the number of syzygies. To make this discussion more concrete, we will discuss explicit examples in the next section. It is worth noting that a similar cancellation was observed in a low-energy neutrino model in Ref. [220], which also corresponds to a non-complete intersection ring. We can understand these cancellations as follows.

For a sufficiently simple invariant ring, the orders in the plethystic logarithm, where negative terms indicating syzygies and positive terms indicating generating invariants appear, are well-separated. As the ring becomes more complicated, either due to a more complicated group structure or due to larger or more involved representations obtained as the tensor product of simple representations, more invariants are needed to describe the full algebraic structure of the ring. Hence, there exist more generating invariants at higher orders and the positive terms in the plethystic logarithm extend to higher orders. Then, assuming that syzygies among the lower-order generating invariants still appear at a similar order as in less complicated rings, there will be an overlap between the regions of positive and negative terms. This overlap results in cancellations between the number of generating invariants and the number of syzygies. Therefore, caution should be taken when using the plethystic logarithm as the sole mean to count the number of generating invariants and the number of syzygies in a non-complete intersection ring. Observing a negative term in the plethystic logarithm does not necessarily imply the absence of generating invariants, but rather indicates the presence of more syzygies than generating invariants. Hence, *the coefficient in the plethystic logarithm is the difference between the number of generating invariants and the number of syzygies.*

There exist further redundancies in the ungraded plethystic logarithm, which can appear due to the overlap of the regions where positive and negative terms appear. The coefficients in the ungraded plethystic logarithm can be subject to cancellations from terms which have a different grading for the same total order in the multi-graded plethystic logarithm but cancel once the ungraded limit is taken. In this sense, we can not naively assume that the leading positive terms in Eq. (3.8) correctly counts all generating invariants as is the case in a complete intersection ring. Hence, the multi-graded plethystic logarithm (see App. 3.B) will be our main guide in what follows to check if the correct number of generating invariants and syzygies was found at a given order in the spurions. We will furthermore assume that the generating invariants are all captured by the terms before the pure negative order[6] in the multi-graded plethystic logarithm, as was conjectured in Ref. [252]. The pure negative terms occur at order 26 in Eq. (3.55) in the νSM, so the *generating* set should only contain invariants up to order 24. However, to test if the conjecture holds true, we also construct invariants up to order 26 to see that indeed no generating invariant can be found at this pure

[6] In the multi-graded plethystic logarithm, we organise the terms according to their order in the ungraded plethystic logarithm. In a given order, if all terms are negative, it is called a *pure negative* order.

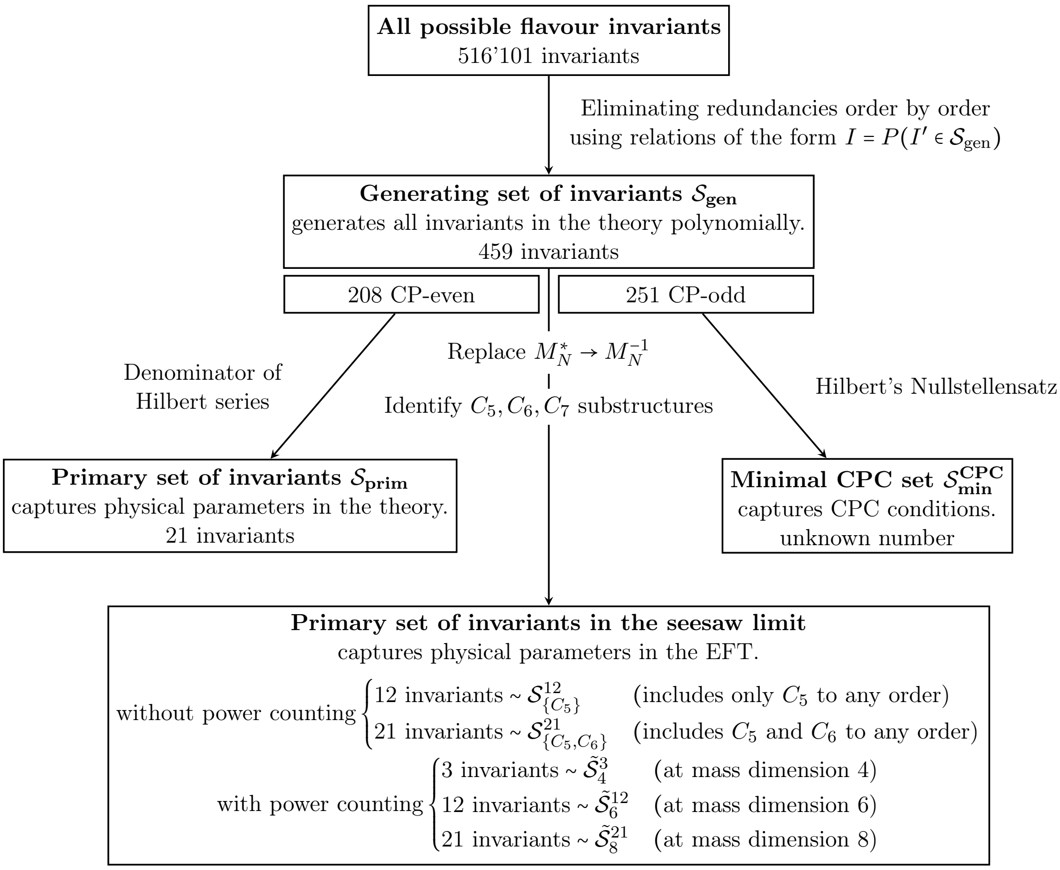


Figure 3.1: Flow graph of different invariant sets that appear in the analysis alongside the algorithms that are used to obtain one set from another. The number in the top box correspond to all single trace invariants up to a total order of 26 in all spurions. We find 208 CP-even and 251 CP-odd invariants that make up the *generating* set of the ring defined by the Lagrangian parameters and their transformation properties. A complete list of these invariants can be found in App. 3.C. The 21 algebraically independent invariants are selected from the CP-even *generating* set to form the *primary* set. These invariants accurately capture the 21 physical parameters of the theory. To determine the CPC conditions, the CP-odd invariants are selected from the CP-odd *generating* set. However, our program fails to find the minimal set due to the complexity of the theory. Detailed explanations on Hilbert's Nullstellensatz can be found in App. 3.D. In the seesaw limit, we replace $M_N^* \to M_N^{-1}$ for the generating invariants, and identify invariants with substructures of C_5, C_6 and C_7 as defined in Eq. (3.17). The number of primary invariants with and without considering the total suppression of the invariants in the heavy Majorana mass is obtained by calculating the Jacobian rank of the identified invariants. A detailed analysis can be found in Sec. 3.3, where the *primary* sets $\mathcal{S}$ and $\tilde{\mathcal{S}}$ are shown explicitly.

negative order. As we will see below, our analysis supports this conjecture.

3.2.2 Constructing the Invariants

Although the plethystic logarithm can be used as a guide regarding the number of generating invariants and their spurion content, their specific form remains unknown. While it is possible to construct invariants manually for some simple models without any further help, in the case of complicated invariant rings like the νSM with hundreds of generating invariants, it becomes unfeasible to construct invariants manually and find the explicit relations among the all possible invariants, which reduce them to the generating set. As mentioned earlier, what

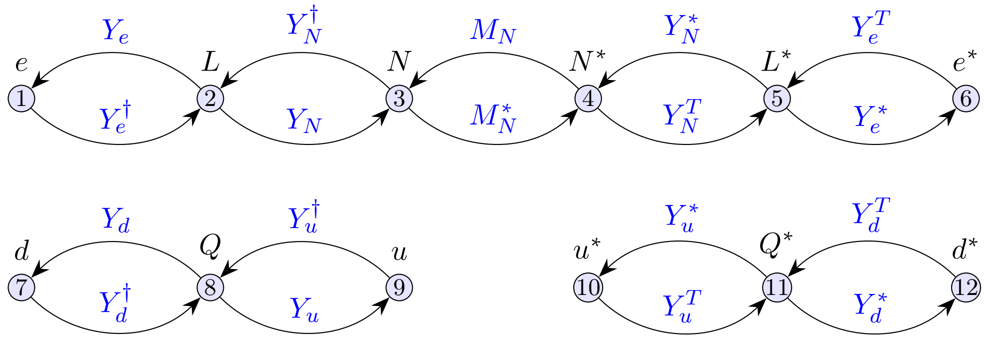
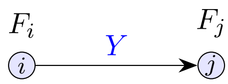


Figure 3.2: The flavour invariant graph that can be used to construct all possible single-trace flavour invariants in the νSM. A single-trace invariant can be associated with any closed walk following the arrows. Note that the graph for the SM has a "holomorphic" structure, i.e., it has two separated branches involving separately only fields or only their conjugates. This changes in the νSM, where the transformation properties of the Majorana mass M_N connect the holomorphic and anti-holomorphic branches. More details can be found in the main text.

complicates things even more in sufficiently complicated invariant rings is, that the orders at which generating invariants and syzygies appear in the plethystic logarithm might overlap, leading to cancellations of terms in the plethystic logarithm. To construct a *generating* set, one therefore cannot solely rely on the information provided by the plethystic logarithm.

Instead, we will start by constructing all possible invariants by brute force up to the first purely negative order, which due to the conjecture presented earlier is the highest order where generating invariants are expected. We perform the construction with a graph-based method, which we will introduce in this section, with the objective of eliminating redundant invariants with explicit relations and creating a *generating* set. Subsequently, we will further reduce this *generating* set to a *primary* set, capturing the physical degrees of freedom of the theory. In a last step, we aim to find the minimal set of invariants that determines the necessary and sufficient condition for CPC, based on the CP-odd generating invariants of the theory. We have summarised this process in a flow graph in Fig. 3.1.

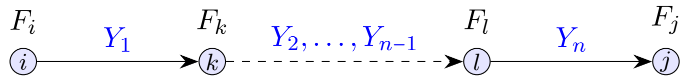
Flavour Invariants from Closed Walks in a Graph To systematically perform the construction of all possible flavour invariants up to the order suggested by the plethystic logarithm, we introduce the concept of the flavour invariant graph, inspired by Ref. [261]. The corresponding graph for the νSM is shown in Fig. 3.2, where the disconnected lepton sector and quark sector are shown in the top and bottom panels, respectively. In each graph, the nodes in the graph are labelled by the fields and their conjugates, which are connected by the flavourful couplings in the theory according to their transformation properties following Tab. 3.1. Following the transformation properties allows to write down the following basic elements of the graph



where the arrow labelled with flavour matrix Y, going from vertex i to vertex j, labelled with the fields F_i and F_j respectively, indicates that the flavour matrix Y transforms as

$Y \to U_{F_i} Y U_{F_j}^\dagger$ under the flavour group. The numbers at the vertices are only for labelling purposes, which will allow us to write down the invariants in a compact form later. F_i should simply be understood as the field at vertex i and should not to be confused with the flavour index of the fermion. As an example, the graph in Fig. 3.2 allows us to read off $Y_e \to U_L Y_e U_e^\dagger$ and $Y_e^* \to U_{L^*} Y_e^* U_{e^*}^\dagger = U_L^* Y_e^* U_e^T$, where we have used that $U_{f^*} = U_f^*$.

Second, following the directional flow of the arrows, allows us to construct covariants under the flavour group, which are matrix products of the simple flavourful couplings of the theory. Passing through the vertices following the arrows, one creates "paths", which if they include repetitions of the same vertices and edges are dubbed "walks" in mathematical terminology. To every walk, one can associate an object with specific transformation under the flavour group. For instance, in the graph below, starting from vertex i and following the sequence of arrows until reaching vertex j,



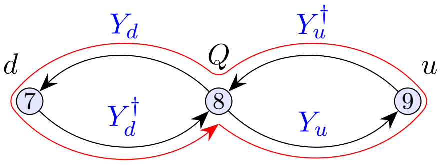
the product of flavour matrices $X \equiv Y_1 \dots Y_n$ will transform as $X \to U_{F_i} X U_{F_j}^\dagger$. To give another example from the νSM, following the graph in Fig. 3.2 we can simply read off that the combination $Y_e^\dagger Y_N$ has the following transformation properties under the flavour group $Y_e^\dagger Y_N \to U_e Y_e^\dagger Y_N U_N^\dagger$.

Finally, we can use the walks to systematically build invariants. This is done by demanding that the walk be closed and ends at its starting vertex. If we choose $i = j$ in the last example, we have $X \to U_{F_i} X U_{F_i}^\dagger$, which allows us to construct the single-trace invariant $\mathrm{Tr}(X)$ under the action of the group. As a result, flavour invariants are mapped to closed walks in the graph, and vice-versa one can identify a closed walk with each single-trace invariant in the theory.[7]

Let us discuss a couple more examples to make this connection clear and familiarise ourselves with the notation. One can construct the following two invariants in the νSM corresponding two invariants in the quark and lepton sectors of the theories (the red paths

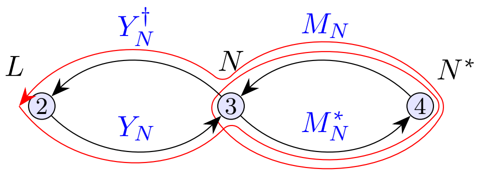
[7] One can also find other forms of flavour invariants, but they can always be mapped to the single-trace invariants presented here [3, 103].

represent closed walks on the graphs denoted by the black arrows connecting the vertices)



$$\sim 8 \to 9 \to 8 \to 7 \to 8$$

$$\sim \mathrm{Tr}\left(Y_u Y_u^\dagger Y_d Y_d^\dagger\right), \tag{3.9}$$



$$\sim 2 \to 3 \to 4 \to 3 \to 4 \to 3 \to 2$$

$$\sim \mathrm{Tr}\left(Y_N M_N^* M_N M_N^* M_N Y_N^\dagger\right).$$

Here, we have given the walks as a chain of numbers corresponding to the vertices that are passed through, which will be convenient later to present the more complicated invariants in a concise way. We only show here simple examples of walks in subsets of the νSM graph. Due to the cyclicity of the trace, the invariant associated to a closed walk is independent of the starting vertex, e.g. $8 \to 9 \to 8 \to 7 \to 8 = 7 \to 8 \to 9 \to 8 \to 7$ for the first example above. Based on this, we will always rotate the numbers in the chain to arrange them in the lexicographically smallest order in the following. Furthermore, since the last vertex in a closed walk is always identical with the first vertex, the last number in the chain can be omitted. To further shorten the notation, the arrow can be removed from the chain of numbers resulting in an integer representation of the walk notation. By following this approach, all single trace invariants are uniquely represented as integers. For instance, the two invariants above are represented by the two integers 7898 and 234343, respectively.

One important difference between the SM and the νSM flavour sector is the inclusion of the Majorana neutrino mass M_N, which connects the parts of the flavour graphs with conjugate fields to the one without conjugate fields (c.f. Fig. 3.2). Indeed, in the quark sector there are two separate parts and closed walks have a "holomorphic" or "anti-holomorphic" structure, i.e. they involve either the fields or their complex conjugate at the vertices, but never mix both. Using the hermiticity of the matrices and trace relations, one can show that the invariants built from both parts of the invariant graph are equivalent (see Ref. [4] for details). The introduction of the Majorana neutrino mass term M_N connects the two conjugate parts, complicating the flavour sector of the theory and allowing for many more independent invariants.

In the Dirac limit, $M_N \to 0$, the flavour structure of the νSM lepton sector reduces to that of the SM quark sector by identifying $Y_N \sim Y_u, Y_e \sim Y_d$, thus their flavour invariants have the same form. We have already constructed the flavour invariants of the SM quark sector in Eq. (2.98), which can be mapped to those of the νSM in the Dirac limit by the replacement $Y_u \to Y_N, Y_d \to Y_e$.

For non-zero and finite M_N, we can systematically enumerate the closed walks corresponding to all single-trace flavour invariants up to arbitrarily high order. In particular, we are interested in the invariants constructed by the walks up to order 26 in the flavour spurions, which is the first pure negative order in the multi-graded plethystic logarithm of the νSM sufficient to obtain a set of generating invariants [252]. The details of the brute-force algorithm utilised to construct all the 516'001 single-trace invariants up to order 26 can be found in Ref. [4]. Among all those single-trace invariants, there are still lots of redundancies, some of which can be immediately removed with the following simple relations.

- Transpose redundancy

  Every walk $W_1 \equiv ij\ldots kl$ in the graph of the νSM is accompanied by another walk with primed vertices in reverse order $W_2 \equiv l'k'\ldots j'i'$, where $v' = 7 - v$ for the graph in the lepton sector. The reversed order walks correspond to the flavour invariants, where the transposed matrix is used for all matrices appearing in the invariant and it can be eliminated with the following trace identity $\mathrm{Tr}\left(A^T\right) = \mathrm{Tr}\left(A\right)$. For instance, $\mathrm{Tr}\left(Y_e Y_e^\dagger\right) = \mathrm{Tr}\left(Y_e^* Y_e^T\right)$.

- Conjugate redundancy

  The walk W_1 defined above is also associated with another walk $W_3 \equiv i'j'\ldots k'l'$. The invariants generated by these two walks are conjugate to each other. Thus, both $\mathrm{Tr}(A)$ and $\mathrm{Tr}(A^*)$ will be generated in our construction. As the CP properties of $\mathrm{Re}\,\mathrm{Tr}(A)$ and $\mathrm{Im}\,\mathrm{Tr}(A)$ are more transparent than those of $\mathrm{Tr}(A)$ and $\mathrm{Tr}(A^*)$, we will trade $\mathrm{Tr}(A)$ and $\mathrm{Tr}(A^*)$, which are generated by the graphs, with $\mathrm{Re}\,\mathrm{Tr}(A)$ and $\mathrm{Im}\,\mathrm{Tr}(A)$, whenever a complex invariant is found.

- Cayley–Hamilton theorem

  The Cayley–Hamilton theorem, along with its simple variations (see Refs. [4, 218]), enables us to eliminate invariants by establishing relations among them. Note that the theorem is not fully utilised here, as there are more complex variations for products of matrices, that are not easy to employ in practice. To remove the remaining redundancies, we will implement a generic numerical algorithm.

The details of the redundancies are discussed in Ref. [4]. After all of these redundancies are eliminated, a set of 8'666 invariants remains, which still has many explicit relations among its invariants and hence does not form a generating set.

Construction of the generating set After prereducing the set of invariants, we systematically construct a generating set order by order in the spurions. To this end, we construct a candidate generating set only containing the lowest order invariants. Then, we add the invariants at the next order to the set and search for explicit relations of these newly added invariants in terms of the other invariants added at lower orders. Whenever an explicit relation is found, the corresponding invariant is removed from our set. When the algorithm has eliminated all explicit redundancies at a given order, it continues constructing relations at the next order including all the invariants that have survived the algorithm up to this point in its preliminary *generating* set, until the maximum order 26 is reached. After the algorithm has completed, all explicit redundancies among the invariants are removed and a generating set of invariants is found. In order to remove all explicit redundancies systematically, we have implemented a numerical algorithm (for details see Ref. [4]), turning the complicated problem of finding polynomial relations among invariants into a problem of solving finite system of linear equations. This algorithm has been used in different forms in Refs. [1, 103, 220, 250] before and was adapted for this work to avoid redundant syzygies[8]. By using this method, we are able to generate all possible polynomial relations among the invariants at each degree, including both explicit relations and syzygies among the generating invariants, which allow us later to verify our numbers of generating invariants and syzygies against the numbers in the plethystic logarithm.

After running the algorithm up to order 26, our final set of generating invariants for the νSM contains 459 invariants, out of which 208 are CP-even and 251 are CP-odd. We want to stress again that any invariant in the νSM can be expressed as a polynomial of these 459 flavour invariants. Hence, as observables should be independent of any mathematical basis, including the flavour basis, they should in principle be expressible in terms of these invariants. In the following sections, we will further reduce the *generating* set to a *primary* set, which captures all physical parameters in the theory. Additionally, we aim to reduce the CP-odd *generating* set to a minimal CPC set, that captures all necessary and sufficient conditions for CPC in the νSM (c.f. Fig. 3.1). The full generating set of invariants, split into its CP-even and CP-odd parts, can be found in Ref. [4]. In the following, we will work with this generating set and label the ith invariant in the CP-even (CP-odd) subset of the generating set by $\mathcal{I}_i (\mathcal{J}_i)$.

Explicit relations and syzygies To verify that our generating set is indeed complete, we can use the numbers in the plethystic logarithm to cross-check them against the numbers of generating invariants and syzygies found in the previous steps. To this end, we require both the number of generating invariants and szyzygies at all orders in the spurions to compute the difference between them which can be compared with the prefactors of the terms in the plethystic logarithm. The algorithm outlined earlier in this section provides all of this information. Here, the most difficult part is to identify the non-redundant syzygies which cannot be expressed as a combination of other syzygies appearing at earlier orders and other generating invariants or syzygies.

To exemplify this step, we show some examples for polynomial relations found by the algorithm, including both explicit relations and syzygies. Our program scans and checks all terms in the plethystic logarithm from lowest to highest order. Prior to order 12, our reduced invariant set exactly reproduces the prefactors of the corresponding terms in the plethystic logarithm. Therefore, no polynomial relations are found up to this order and all invariants up to this point are generating invariants. At degree $e^6 n^6$ in the spurions, two invariants are found in our pre-reduced set, given by $\mathcal{I} \equiv \mathrm{Re}\,\mathrm{Tr}\left(X_N^2 X_e^2 X_N X_e\right)$ and $\mathcal{J}_{10} \equiv \mathrm{Im}\,\mathrm{Tr}\left(X_N^2 X_e^2 X_N X_e\right)$, where X_N and X_e are defined in Tab. 3.1, but the corresponding term in the multi-graded

[8] Redundant syzygies are those which have previously appeared in the algorithm at a lower order in the spurions and are multiplied by another syzygy, which has previously appeared, or some invariant of the *generating* set (or a sum of both), hence reappearing at a higher order. These kind of syzygies evidently do not carry any new information. This is also discussed in Ref. [250], where the term “old relation” is used.

plethystic logarithm in Eq. (3.55) has the following form $+e^6 n^6$. Therefore, either one of the invariants must be expressible as a polynomial of all previous invariants in the set, hence is not a generating invariant, or there exists a syzygy at the order leading to a cancellation with the number of generating invariants. Indeed, our algorithm finds an explicit relation, which allows us to rewrite the CP-even invariant $\mathcal{I}$ as a polynomial of other lower-degree CP-even invariants

$$
\begin{aligned}
6\mathcal{I} = {} & \mathcal{I}_3^3\mathcal{I}_1^3 - \mathcal{I}_3\mathcal{I}_6\mathcal{I}_1^3 - 3\mathcal{I}_3^2\mathcal{I}_7\mathcal{I}_1^2 + 3\mathcal{I}_3\mathcal{I}_{12}\mathcal{I}_1^2 - \mathcal{I}_3^3\mathcal{I}_4\mathcal{I}_1 + \mathcal{I}_4\mathcal{I}_{11}\mathcal{I}_1 + \\
& + 3\mathcal{I}_3^2\mathcal{I}_{13}\mathcal{I}_1 - 3\mathcal{I}_3\mathcal{I}_{18}\mathcal{I}_1 + \mathcal{I}_3\mathcal{I}_6\mathcal{I}_9 - \mathcal{I}_9\mathcal{I}_{11} + 3\mathcal{I}_{12}\mathcal{I}_{13} + 3\mathcal{I}_7\mathcal{I}_{18}\,.
\end{aligned}
\tag{3.10}
$$

Hence, the CP-even invariant is redundant, while no explicit relation for the CP-odd invariant $\mathcal{J}_{10}$ and no syzygies for the lower order invariants can be found at the same order. As a consequence, we can successfully reproduce the number in the plethystic logarithm.

Finding this cancellation was expected, as $\mathcal{J}_{10}$ is the equivalent of the Jarlskog invariant in the lepton sector obtained by exchanging all quark Yukawa couplings with the corresponding lepton Yukawa coupling and its related CP-even invariant is known to be redundant [218]. Note, that $\mathcal{J}_{10}$ is the only CP-odd generating invariant in the νSM that has no dependence on M_N, consistent with the fact that there is only a single new source of CP violation in the νSM for conservation of lepton number.

Running our algorithm up to order 14, the number of generating invariants agrees with the numbers indicated by the prefactors in the multi-graded plethystic logarithm. Only at degree $m^8 n^8$, we run into another mismatch. At this order, there exist a total of 10 invariants in the pre-reduced set, but we only find 9 explicit relations. As a result, we are left with one invariant $\mathcal{J}_{76}$ that cannot be written as any polynomial of other invariants and hence should be identified as a *generating* invariant. However, there exists no term in the multi-graded plethystic logarithm in Eq. (3.55) at degree $m^8 n^8$, suggesting that no generating invariants exist at this order. But, as we mentioned in Sec. 3.2.1, there can be non-trivial cancellations between the number of generating invariants and syzygies. Indeed, we also find another relation at degree $m^8 n^8$, which is given by

$$
\begin{aligned}
& 3\mathcal{I}_5^2\mathcal{I}_3^4 - 3\mathcal{I}_2\mathcal{I}_{10}\mathcal{I}_3^4 - 8\mathcal{I}_2^3\mathcal{I}_8\mathcal{I}_3^3 + 12\mathcal{I}_2\mathcal{I}_5\mathcal{I}_8\mathcal{I}_3^3 + 8\mathcal{I}_8\mathcal{I}_{10}\mathcal{I}_3^3 + 12\mathcal{I}_2^2\mathcal{I}_{16}\mathcal{I}_3^3 - 24\mathcal{I}_5\mathcal{I}_{16}\mathcal{I}_3^3 + \\
& + 30\mathcal{I}_2^2\mathcal{I}_8^2\mathcal{I}_3^2 - 18\mathcal{I}_5\mathcal{I}_8^2\mathcal{I}_3^2 + 36\mathcal{I}_{16}^2\mathcal{I}_3^2 - 6\mathcal{I}_5^2\mathcal{I}_6\mathcal{I}_3^2 + 6\mathcal{I}_2\mathcal{I}_6\mathcal{I}_{10}\mathcal{I}_3^2 + 8\mathcal{I}_2^3\mathcal{I}_{14}\mathcal{I}_3^2 - 12\mathcal{I}_2\mathcal{I}_5\mathcal{I}_{14}\mathcal{I}_3^2 + \\
& - 8\mathcal{I}_{10}\mathcal{I}_{14}\mathcal{I}_3^2 + 10\mathcal{I}_2^3\mathcal{I}_{15}\mathcal{I}_3^2 - 18\mathcal{I}_2\mathcal{I}_5\mathcal{I}_{15}\mathcal{I}_3^2 - 4\mathcal{I}_{10}\mathcal{I}_{15}\mathcal{I}_3^2 - 60\mathcal{I}_2\mathcal{I}_8\mathcal{I}_{16}\mathcal{I}_3^2 - 12\mathcal{I}_2^2\mathcal{I}_{20}\mathcal{I}_3^2 + \\
& + 24\mathcal{I}_5\mathcal{I}_{20}\mathcal{I}_3^2 - 24\mathcal{I}_2^2\mathcal{I}_{21}\mathcal{I}_3^2 + 24\mathcal{I}_5\mathcal{I}_{21}\mathcal{I}_3^2 + 24\mathcal{I}_2\mathcal{I}_{28}\mathcal{I}_3^2 - 24\mathcal{I}_2\mathcal{I}_8^3\mathcal{I}_3 + 8\mathcal{I}_2^3\mathcal{I}_6\mathcal{I}_8\mathcal{I}_3 + \\
& - 12\mathcal{I}_2\mathcal{I}_5\mathcal{I}_6\mathcal{I}_8\mathcal{I}_3 - 8\mathcal{I}_6\mathcal{I}_8\mathcal{I}_{10}\mathcal{I}_3 - 24\mathcal{I}_2^2\mathcal{I}_8\mathcal{I}_{14}\mathcal{I}_3 + 24\mathcal{I}_5\mathcal{I}_8\mathcal{I}_{14}\mathcal{I}_3 - 48\mathcal{I}_2^2\mathcal{I}_8\mathcal{I}_{15}\mathcal{I}_3 + 24\mathcal{I}_5\mathcal{I}_8\mathcal{I}_{15}\mathcal{I}_3 + \\
& + 48\mathcal{I}_8^2\mathcal{I}_{16}\mathcal{I}_3 - 12\mathcal{I}_2^2\mathcal{I}_6\mathcal{I}_{16}\mathcal{I}_3 + 24\mathcal{I}_5\mathcal{I}_6\mathcal{I}_{16}\mathcal{I}_3 + 24\mathcal{I}_2\mathcal{I}_{14}\mathcal{I}_{16}\mathcal{I}_3 + 48\mathcal{I}_2\mathcal{I}_{15}\mathcal{I}_{16}\mathcal{I}_3 - 16\mathcal{I}_2^3\mathcal{I}_{19}\mathcal{I}_3 + \\
& + 24\mathcal{I}_2\mathcal{I}_5\mathcal{I}_{19}\mathcal{I}_3 + 16\mathcal{I}_{10}\mathcal{I}_{19}\mathcal{I}_3 + 48\mathcal{I}_2\mathcal{I}_8\mathcal{I}_{20}\mathcal{I}_3 - 48\mathcal{I}_{16}\mathcal{I}_{20}\mathcal{I}_3 + 48\mathcal{I}_2\mathcal{I}_8\mathcal{I}_{21}\mathcal{I}_3 - 48\mathcal{I}_{16}\mathcal{I}_{21}\mathcal{I}_3 + \\
& + 48\mathcal{I}_2^2\mathcal{I}_{27}\mathcal{I}_3 - 48\mathcal{I}_5\mathcal{I}_{27}\mathcal{I}_3 - 48\mathcal{I}_8\mathcal{I}_{28}\mathcal{I}_3 - 48\mathcal{I}_2\mathcal{I}_{39}\mathcal{I}_3 + 3\mathcal{I}_5^2\mathcal{I}_6^2 - 6\mathcal{I}_2^2\mathcal{I}_6\mathcal{I}_8^2 + 6\mathcal{I}_5\mathcal{I}_6\mathcal{I}_8^2 + 6\mathcal{I}_2^2\mathcal{I}_{14}^2 + \\
& - 6\mathcal{I}_5\mathcal{I}_{14}^2 + 24\mathcal{I}_2^2\mathcal{I}_{15}^2 - 12\mathcal{I}_5\mathcal{I}_{15}^2 - 12\mathcal{I}_6\mathcal{I}_{16}^2 + 24\mathcal{I}_{20}^2 + 12\mathcal{I}_{21}^2 - 3\mathcal{I}_2\mathcal{I}_6^2\mathcal{I}_{10} + 12\mathcal{I}_2\mathcal{I}_8^2\mathcal{I}_{14} + \\
& + 24\mathcal{I}_2\mathcal{I}_8^2\mathcal{I}_{15} - 10\mathcal{I}_2^3\mathcal{I}_6\mathcal{I}_{15} + 18\mathcal{I}_2\mathcal{I}_5\mathcal{I}_6\mathcal{I}_{15} + 4\mathcal{I}_6\mathcal{I}_{10}\mathcal{I}_{15} + 12\mathcal{I}_2\mathcal{I}_6\mathcal{I}_8\mathcal{I}_{16} - 24\mathcal{I}_8\mathcal{I}_{14}\mathcal{I}_{16} + \\
& - 24\mathcal{I}_8\mathcal{I}_{15}\mathcal{I}_{16} + 24\mathcal{I}_2^2\mathcal{I}_8\mathcal{I}_{19} - 24\mathcal{I}_5\mathcal{I}_8\mathcal{I}_{19} - 24\mathcal{I}_2\mathcal{I}_{16}\mathcal{I}_{19} - 24\mathcal{I}_8^2\mathcal{I}_{20} + 12\mathcal{I}_2^2\mathcal{I}_6\mathcal{I}_{20} - 24\mathcal{I}_5\mathcal{I}_6\mathcal{I}_{20} +
\end{aligned}
\tag{3.11}
$$

$$-48\mathcal{I}_2\mathcal{I}_{15}\mathcal{I}_{20}-24\mathcal{I}_2\mathcal{I}_{14}\mathcal{I}_{21}+6\mathcal{I}_2^3\mathcal{I}_{26}-6\mathcal{I}_2\mathcal{I}_5\mathcal{I}_{26}-12\mathcal{I}_{10}\mathcal{I}_{26}-48\mathcal{I}_2\mathcal{I}_8\mathcal{I}_{27}+48\mathcal{I}_{16}\mathcal{I}_{27}+$$
$$+24\mathcal{I}_{14}\mathcal{I}_{28}-24\mathcal{I}_2^2\mathcal{I}_{38}+24\mathcal{I}_5\mathcal{I}_{38}+48\mathcal{I}_8\mathcal{I}_{39}+24\mathcal{I}_2\mathcal{I}_{55}+12\mathcal{J}_1^2=0\,,$$

As no invariant enters linearly in this polynomial relation, it is a syzygy among lower-order invariants – not an explicit redundancy of an invariant. It only depends on the square of a single CP-odd invariant $\mathcal{J}_1^2$ and can therefore be interpreted in the same way as the syzygy of the Jarlskog invariant in the SM quark sector, presented in Sec. 2.5.1. It states that $\mathcal{J}_1$ only gives information about the sign of the corresponding phase, its magnitude is already captured by another CP-even invariant. Therefore, the square of $\mathcal{J}_1$ does not contain any additional information and should be expressible in terms of other invariants.

Hence, combining the two findings we have

$$\mathrm{PL}\,(e,m,n)\supset +m^8n^8-m^8n^8\,, \tag{3.12}$$

explaining the non-trivial zero in the plethystic logarithm. At higher degrees in the spurions even stronger cancellations appear, that can even generate negative terms at orders where a (large) number of generating invariants exist. Some examples are

$$\mathrm{PL}\,(e,m,n)\supset(21-1)\,e^4m^4n^8+(3-1)\,e^2m^4n^{12}+(3-6)\,e^2m^6n^{10}+(2-6)\,e^2m^8n^8\,, \tag{3.13}$$

where we have used (n_g-n_s) as a coefficient to indicate the n_g generating invariants and n_s syzygies at the corresponding degree.

Although there may be challenges when identifying generating invariants and syzygies, as long as the terms in the plethystic logarithm are correctly interpreted, we are able to determine the correct number of the generating invariants and syzygies at each degree. Our algorithm accurately generates the terms in the plethystic logarithm up to order 24 based on the new interpretation of the plethystic logarithm. However, at order 26, there are some mismatches due to "redundant syzygies", which are not simply products of syzygies that appeared at a lower order in the spurions. We discuss how to address these mismatches in detail in Ref. [4]. The order 26 is the first order that only has negative terms in the multi-graded plethystic logarithm. We have also confirmed that there are no further generating invariants at this order, as all the invariants are found to be a polynomial of lower order invariants.

We have carefully cross-checked the number of generating invariants and the syzygies among them at each degree of $[emn]$ with the terms in the multi-graded plethystic logarithm shown in Eq. (3.55), finding agreement for all of them. We want to stress again that the coefficients of all terms in the plethystic logarithm in this new interpretation should be presented as (n_g-n_s) as shown and described around Eq. (3.13). According to the new multi-graded plethystic logarithm, one can easily read off the correct number of generating invariants and syzygies at each degree. Due to its length, we will not show the plethystic logarithm in this new form here but it can be found in a table in Ref. [4] and the counting for the ungraded orders is presented in Tab. 3.3. With this table, the ungraded plethystic logarithm shown in

Order		2	4	6	8	10	12	14	16	18	20	22	24	26	Total
Gen.	CP-even	3	5	9	8	12	17	25	33	41	34	17	4	0	208
	CP-odd	0	0	0	2	7	23	41	61	61	42	13	1	0	251
Syz.		0	0	0	0	0	0	0	2	32	200	733	2044	4391	7402
PL=Gen.−Syz.		3	5	9	10	19	40	66	92	70	−124	−703	−2039	−4391	−6943

Table 3.3: The number of generating invariants and syzygies from order 2 to order 26, where the generating invariants are split into CP-even and CP-odd in the counting. The difference between the number of generating invariants and number of syzygies precisely aligns with the terms in the ungraded plethystic logarithm shown in Eq. (3.8). In the last column, we list the total number of CP-even, CP-odd generating invariants, syzygies, and their difference. In the complete intersection ring, the difference between the number of generating invariants and number of syzygies should be the Krull dimension, which is 21 in our theory. The negative number shown here featuring a non-complete intersection ring.

Eq. (3.8) can be rewritten as follows

$$\begin{aligned} \mathrm{PL}[\mathcal{H}(q)] = \; & (3-0)\,q^2 + (5-0)\,q^4 + (9-0)\,q^6 + (10-0)\,q^8 + (19-0)\,q^{10} + (40-0)\,q^{12} \\ & +(66-0)\,q^{14} + (94-2)\,q^{16} + (102-32)\,q^{18} + (76-200)\,q^{20} \\ & +(30-733)\,q^{22} + (5-2044)\,q^{24} + (0-4391)\,q^{26} + \mathcal{O}(q^{28})\,. \end{aligned} \tag{3.14}$$

Comparing with Eq. (3.8), one can easily see that the coefficients in the plethystic logarithm computed there are exactly the same as those shown here.

At higher orders, the coefficients in the plethystic logarithm can no longer be connected to meaningful quantities like the number of generating invariants or the number of syzygies at a given degree [220, 223]. For instance, at order 28, we can find two positive terms

$$\mathrm{PL}\,(e,m,n) \supset +6m^{14}n^{14} + 4m^{16}n^{12}\,. \tag{3.15}$$

However, all invariants constructed by brute force at these two degrees are redundant after applying the Cayley–Hamilton theorem. Therefore, there is no generating invariant, and these two positive terms are meaningless.[9] We have also checked this explicitly by constructing the invariants at order 26 and checking that they can be expressed as polynomials of the generating set. Hence, we are confident that the algorithm can be terminated at the first pure negative order 24, as conjectured in Ref. [220]. Note, that identifying all independent syzygies at each order is technically not necessary to obtain the *generating*, for which it is sufficient to construct the explicit relations. Additionally counting the syzygies is only necessary, if the plethystic logarithm is used to cross-check the number of generating invariants.

[9] All terms in the non-terminating plethystic logarithm of a non-complete intersection ring after the leading negative terms have – to our knowledge – no meaning for the construction of a *generating* set beyond the fact that they appear in a special form of the Hilbert series, the so-called Euler form [223]. In this form the Hilbert series can be written as $\mathcal{H}(q) = \prod_{n=1}^{\infty}(1-q^n)^{-b_n}$, where it can be shown that the b_n are exactly the coefficients in the plethystic logarithm $\mathrm{PL}\,[\mathcal{H}\,(q)] = \sum_{n=1}^{\infty} b_n q^n$.

3.2.3 A Primary Set for the νSM

The next step after identifying the generating set is to reduce it to a *primary* set of algebraically independent invariants, that captures all physical parameters of the theory. To simplify this task, we can use the denominator of the Hilbert series as a guide, but in principle any algebraically independent subset of the generating set works as a primary set. The invariants of the primary set capture all physical parameters in the theory. In order to keep redundancies at a minimum from the start, we choose the candidate sets with cardinalities equal to 21, which is the number of physical parameters in the case of the νSM. One way to check if a candidate set is algebraically independent is to calculate the Jacobian with respect to all parameters in a given parameterisation of the Lagrangian, for which we will use the algebraic parameterisation from Eq. (3.47). If the rank of the Jacobian is equal to the number of physical parameters in the theory, a set of algebraically independent invariants is found. Following this procedure we find the following *primary* set

$$\begin{aligned}
&\mathcal{I}_1 = \mathrm{Tr}\left(X_e\right),\ \mathcal{I}_2 = \mathrm{Tr}\left(X_M\right),\ \mathcal{I}_3 = \mathrm{Tr}\left(X_N\right),\ \mathcal{I}_5 = \mathrm{Tr}\left(X_M^2\right),\ \mathcal{I}_6 = \mathrm{Tr}\left(X_N^2\right),\\
&\mathcal{I}_7 = \mathrm{Tr}\left(X_e X_N\right),\ \mathcal{I}_8 = \mathrm{Tr}\left(Z_{MN}\right),\ \mathcal{I}_9 = \mathrm{Tr}\left(X_e^3\right),\ \mathcal{I}_{12} = \mathrm{Tr}\left(X_e X_N^2\right),\ \mathcal{I}_{13} = \mathrm{Tr}\left(X_e^2 X_N\right),\\
&\mathcal{I}_{15} = \mathrm{Tr}\left(X_N Z_{MN}\right),\ \mathcal{I}_{23} = \mathrm{Re}\,\mathrm{Tr}\left(X_e X_N Z_{MN}\right),\ \mathcal{I}_{25} = \mathrm{Tr}\left(X_e^2 Z_{MN}\right),\\
&\mathcal{I}_{34} = \mathrm{Tr}\left(X_e^2 Y_N M_N^* Y_N^T Y_N^* M_N Y_N^\dagger\right),\ \mathcal{I}_{35} = \mathrm{Tr}\left(X_e Y_N M_N^* Y_N^T X_e^* Y_N^* M_N Y_N^\dagger\right),\\
&\mathcal{I}_{47} = \mathrm{Tr}\left(X_e^2 Y_N M_N^* Y_N^T X_N^* Y_N^* M_N Y_N^\dagger\right),\ \mathcal{I}_{50} = \mathrm{Re}\,\mathrm{Tr}\left(X_e X_N Y_N M_N^* Y_N^T X_e^* Y_N^* M_N Y_N^\dagger\right),\\
&\mathcal{I}_{54} = \mathrm{Tr}\left(X_e^2 Y_N M_N^* Y_N^T X_e^* Y_N^* M_N Y_N^\dagger\right),\ \mathcal{I}_{65} = \mathrm{Re}\,\mathrm{Tr}\left(X_e^2 X_N^2 Y_N M_N^* Y_N^T Y_N^* M_N Y_N^\dagger\right),\\
&\mathcal{I}_{79} = \mathrm{Tr}\left(X_e^2 Y_N M_N^* Y_N^T X_e^{*2} Y_N^* M_N Y_N^\dagger\right),\ \mathcal{I}_{91} = \mathrm{Re}\,\mathrm{Tr}\left(X_e^2 X_N^2 Y_N M_N^* M_N M_N^* Y_N^T Y_N^* M_N Y_N^\dagger\right),
\end{aligned} \tag{3.16}$$

where $\mathcal{I}_i$ is the ith invariant in the CP-even set presented in Ref. [4], and we have defined $X_e = Y_e Y_e^\dagger, X_N = Y_N Y_N^\dagger, X_M = M_N M_N^*$ and $Z_{MN} = Y_N M_N^* M_N Y_N^\dagger$. We want to stress again, that the set of algebraically independent invariants is not unique. In particular, there are many sets that are compatible with the denominator of the ungraded Hilbert series and have a Jacobian rank of 21. As was mentioned earlier, the Hilbert series does not have a unique form, which also reflects the freedom in choosing a primary set of invariants. For our set of primary invariants, we have only chosen to only include CP-even invariants from the *generating* set. However, it is also possible to include CP-odd invariants, provided they are algebraically independent, which is for instance done for the seesaw effective field theory in Ref. [257]. It might sound strange at first that CP-even invariants can be used to capture CP-violating parameters of the theory. However, the primary invariants only capture the absolute value of the physical parameters. Hence, the sign of the phases in the theory are *not* described by the primary invariants. This is a well-known result in the quark sector of the SM [218], where the Jarlskog invariant has to be added to the set of primary invariants to complete the *generating* set of invariants, enabling the expression of all observables in the theory in terms of flavour invariants. As already explained earlier, the square of the Jarlskog invariant, i.e., the square of the sign of the CKM phase, is in turn expressible in terms of CP-even invariants in agreement with the statement that the square of a sign is trivial.

In addition, we have chosen the orders of the invariants in our *primary* set to follow those of the denominator of the Hilbert series in Eq. (3.7). For instance, the first term $(1-q^2)^3$ of the denominator in Eq. (3.7) indicates that there should be 3 invariants of order 2. However, following our discussion in footnote 5, one can change the numbers in the denominator of the Hilbert series by multiplying the numerator and denominator of it with the same factor $(1+q^k)^m$. In this case, other algebraically independent subsets of the *generating* set with cardinality 21 can function as a *primary* set.

3.3 The Seesaw Limit

The flavour structure of the νSM also captures that of the type-I seeaw model, assuming that instead of the mass being light we take the seesaw limit, where M_N is taken to be much larger than the electroweak scale v, allowing for an EFT description of the model. In this scenario, the heavy neutrinos can be integrated out for which we match the model to the low-energy effective theory with only the light left-handed SM neutrinos. The seesaw limit can be captured by the invariants presented in this chapter by making the observation that M_N^{-1}, appearing in the EFT description, transforms in the same representation as M_N^*. Hence, by replacing $M_N^* \to M_N^{-1}$ we can recycle the invariants presented here to analyse this limit. After the replacement several flavour structures appear in the invariants, which can all be identified with the matching to Wilson coefficients at different orders in the EFT. In particular, we have [80, 262]

$$\begin{aligned} \frac{C_5}{\Lambda} &\sim Y_N M_N^{-1} Y_N^T \,, \\ \frac{C_6}{\Lambda^2} &\sim Y_N (M_N^* M_N)^{-1} Y_N^\dagger \,, \\ \frac{C_7}{\Lambda^3} &\sim Y_N (M_N M_N^* M_N)^{-1} Y_N^T \,, \\ &\vdots \end{aligned} \tag{3.17}$$

where C_5, C_6 and C_7 are the Wilson coefficients of the Weinberg operator [63], the operator $\mathcal{O}_{Hl}^{(1)}$ in the Warsaw basis [87] and the operator $\mathcal{O}_{lHD}^{(2)}$ in Ref. [88], respectively.[10]

As before, it is useful to work with the invariant graphs to get an insight into which kind of structures can appear in the flavour invariants. The relevant graph for the theory in the see limit is shown in Fig. 3.3. The graph features two types of Wilson coefficients C_{LL^T} and $C_{LL^\dagger}$ as an example, where $C_{LL^T} \to U_L C_{LL^T} U_L^T$ and $C_{LL^\dagger} \to U_L C_{LL^\dagger} U_L^\dagger$ respectively. In our case, $C_{LL^T} \sim C_5, C_7$ and $C_{LL^\dagger} \sim C_6$. This shows that the graph approach serves as a general method for constructing flavour invariants and proves to be useful in both UV and EFT studies. Furthermore, the graph in the EFT allows for a clearer understanding of the structure of the invariants. For instance, whenever invariants in the EFT with the Wilson

[10] Note, that at mass dimensions higher than 5, there are other operators that can appear in the matching. $\mathcal{O}_{Hl}^{(1)}$ at dimension-6 and $\mathcal{O}_{lHD}^{(2)}$ at dimension-7 are only examples of an operator that receives a contribution from the matching of the νSM to the SMEFT [262]. Our choice of Wilson coefficients ensures the lowest overall suppression of the invariants with the Majorana mass.

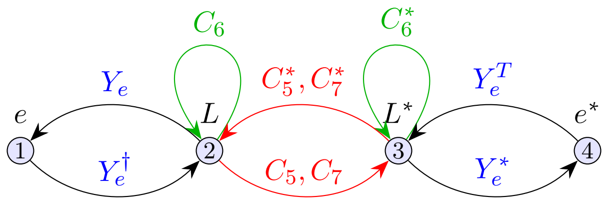


Figure 3.3: The flavour invariant graph that can be used to construct all possible single trace flavour invariants in the seesaw limit of the νSM, where C_5, C_6 and C_7 are the Wilson coefficients of the Weinberg operator [63], the operator $\mathcal{O}_{Hl}^{(1)}$ in the Warsaw basis [87] and the operator $\mathcal{O}_{lHD}^{(2)}$ in Ref. [88], respectively, and they transform as $C_{5,7} \to U_L C_{5,7} U_L^T$ and $C_6 \to U_L C_6 U_L^\dagger$. We show in the main text that it is sufficient to consider C_5, C_6 and C_7 to capture all parameters of the full theory.

coefficient C_5 are constructed, a closed walk in the graph can only be obtained when C_5^* is also included. Following this conclusion, it becomes clear that all constructed invariants are suppressed with an even number of inverse Majorana masses.

We can make several interesting observations with our generating set of invariants in the seesaw limit. Keeping only the invariants with the least suppressed EFT structure corresponding to C_5 as well as Y_e, computing the rank of the Jacobian with respect to all parameters in a chosen parameterisation, yields a rank of 12. This corresponds to the six masses, three mixing angles and three phases that appear in the low-energy theory of three flavours of charged leptons and the left-handed SM neutrinos with a Majorana mass term $\mathcal{L} \supset -1/2\, \bar{\nu}_L m_\nu \nu_L^c + \text{H.c.}$. Out of all invariants surviving in the seesaw limit, there are a total of 15 invariants, containing only C_5 alongside Y_e. Among them, a set of 12 algebraically independent invariants is given by the following invariants

$$\mathcal{S}^{12}_{\{C_5\}} \equiv \{\mathcal{I}_1', \mathcal{I}_4', \mathcal{I}_9', \mathcal{I}_{14}', \mathcal{I}_{22}', \mathcal{I}_{34}', \mathcal{I}_{35}', \mathcal{I}_{54}', \mathcal{I}_{79}', \mathcal{J}_{101}', \mathcal{J}_{168}', \mathcal{J}_{221}'\}\,, \tag{3.18}$$

where $\mathcal{I}_i'(\mathcal{J}_i')$ can be obtained from our generating invariants $\mathcal{I}_i(\mathcal{J}_i)$ (c.f. list in Ref. [4]) by the replacement $M_N^* \to M_N^{-1}$. We introduce the notation $\mathcal{S}_c^r$ to indicate that we only keep invariants with structures c, yielding a rank-r primary invariant set.

If we include invariants with structures corresponding to C_6 in Eq. (3.17) in addition to the previous case, we find that the rank of the Jacobian of the invariants increases to 21, in agreement with the total number of physical parameters in the νSM. We choose the *primary* set to be

$$\mathcal{S}^{21}_{\{C_5,C_6\}} \equiv \mathcal{S}^{12}_{\{C_5\}} \cup \{\mathcal{I}_8', \mathcal{I}_{17}', \mathcal{I}_{25}', \mathcal{J}_{20}', \mathcal{J}_{58}', \mathcal{J}_{62}', \mathcal{J}_{124}', \mathcal{J}_{125}', \mathcal{J}_{189}'\}\,. \tag{3.19}$$

This has previously been noted in Ref. [257], where this analysis is performed in the effective theory of the seesaw model. There, the authors claim that the physical parameters of the full theory can be fully described with flavour invariants of the EFT by only keeping structures in the invariants corresponding to the Wilson coefficient C_5 and C_6. Here, we come to the same conclusion in the full theory of the νSM.

Note that, up to now we have not considered the power counting of the effective theory, i.e., we allowed for invariants with several insertions of the C_5 structure to obtain the ranks of 12 and 21 without adding any higher order Wilson coefficients which could appear at the same order in the power counting. Indeed, working in the effective theory by taking the seesaw limit, one should work consistently to a certain order in the power counting of the theory, which in the EFT of the seesaw model is defined by the characteristic scale of the process divided by the Majorana mass. By counting the number of insertions of M_N consistent with the power counting of the EFT, we find that one cannot reach rank 12 and 21 at dimension 5 and 6, respectively. Instead, without any insertions of M_N, one can reach rank three, corresponding to the masses of the charged leptons with the following primary set

$$\tilde{\mathcal{S}}_4^3 \equiv \{\mathcal{I}'_1, \mathcal{I}'_4, \mathcal{I}'_9\}\,, \tag{3.20}$$

where $\tilde{\mathcal{S}}_d^r$ is the rank-r *primary* set of invariants at mass dimension d. At mass dimension 6, i.e. with 2 insertions of M_N, rank 12 can be reached, for which we construct the following primary set

$$\tilde{\mathcal{S}}_6^{12} \equiv \tilde{\mathcal{S}}_4^3 \cup \{\mathcal{I}'_8, \mathcal{I}'_{14}, \mathcal{I}'_{17}, \mathcal{I}'_{22}, \mathcal{I}'_{25}, \mathcal{I}'_{34}, \mathcal{I}'_{35}, \mathcal{I}'_{54}, \mathcal{I}'_{79}\}\,. \tag{3.21}$$

At dimension 8, i.e. with 4 insertions of M_N, one can reach rank 21, with the following primary set

$$\tilde{\mathcal{S}}_8^{21} \equiv \tilde{\mathcal{S}}_6^{12} \cup \{\mathcal{I}'_{16}, \mathcal{I}'_{21}, \mathcal{I}'_{24}, \mathcal{I}'_{32}, \mathcal{I}'_{37}, \mathcal{I}'_{51}, \mathcal{I}'_{53}, \mathcal{I}'_{78}, \mathcal{I}'_{112}\}\,. \tag{3.22}$$

This set also includes invariants with the structure of C_7. Hence, even though all the information about the νSM is in principle contained in the Wilson coefficients C_5 and C_6, this information can only be accessed in a flavour invariant way at higher mass dimensions. Considering the power counting of the theory, full rank is first reached at dimension 8 by also considering the structure of C_7 in the invariants instead of going to higher mass dimensions beyond dimension 8 by only including the structures of the Wilson coefficients C_5 and C_6. We have summarised the results in the bottom panel of Fig. 3.1.

3.4 Conditions for CP Conservation

The Jarlskog invariant of the SM quark sector is well-established as the order parameter of perturbative CP violation in the SM. As such, it captures all possible ways of perturbatively conserving CP in the SM as its roots, not only including vanishing phases but also cases of degenerate masses or texture zeros in the CKM matrix, which make the CKM phase unphysical and removable from the Lagrangian. In the same spirit we aspire to find a minimal set of Jarlskog-like CP-odd invariants which capture all CPC conditions in the νSM.

Some previous work in this direction has been completed in the literature for the νSM with different numbers of lepton flavours. In Ref. [218], the *generating* set for the νSM with only two generations of right-handed neutrinos and charged leptons ($n_N = n_f = 2$) has been shown, but the discussion of CPC conditions has not been expanded on. In Ref. [252], the minimal seesaw model with two generations of right-handed neutrinos and three generations of charged leptons ($n_N = 2, n_f = 3$) has been discussed. However, the discussion of CPC conditions is provided only with some assumptions about the parameter spectrum. For the three-generation case ($n_N = n_f = 3$), the discussion of CPC conditions is still lacking, as the *generating* set has not been constructed, although the Hilbert series has been calculated in

Refs. [224, 257]. In Ref. [246], without using the Hilbert series and explicit construction of the *generating* set, six CP-odd invariants are provided to characterise CPV effects of the three generation case. Also there, assumptions are made regarding the parameter spectrum of the theory.

Another advantage of the flavour invariants is that they incorporate all CPC conditions as their roots. Hence, they can be used to obtain the conditions even in complicated theories where some conditions are sometimes hard to identify using symmetry arguments. One such example is the case of pseudoreal couplings,[11] which we present for the νSM with 2 generations of leptons in App. 3.E. There, it turns out that even though the theory has irremovable phases, it is still CP-conserving given that a polynomial relation among parameters of the theory is fulfilled. This polynomial relation is one of the roots of the invariants but is impossible to obtain from symmetry arguments. As a result, studying CPC conditions through the generating CP-odd invariants provides a more reliable approach. In the following, we will define the minimal invariant set that captures the CPC conditions, and propose useful methods to find it. However, due to the complexity of the invariant structure of the νSM, finding the proposed minimal set in general can be challenging. The main goal of this section is to establish a framework for studying the CPC conditions, with the final solutions to these sets left for future work.

The CP-odd invariants in the *generating* set $\mathcal{S}_{\text{gen}}$ act as generators of all CPV observables. The vanishing of these invariants establishes the necessary and sufficient conditions for CP conservation in the theory. However, the CP-odd *generating* set does not necessarily have to be the minimal set with this property. The CP-odd *generating* set is required to generate any value of the CP-odd invariants in a given parameterisation, while the set that can determining the presence of CPV only needs to capture all ways of conserving CP in its roots. In principle, the latter set should be a subset of the CP-odd *generating* set, and from now on, we will call it the CPC set. We will call a CPC set with the minimal amount of invariants while still having all the properties of such a set, the minimal CPC set $\mathcal{S}_{\text{min}}^{\text{CPC}}$.

By definition, the minimal CPC set captures all CPC conditions as roots of its invariants and all other CP-odd invariants in the generating set vanish automatically on these roots

$$\mathcal{J}_{\text{min}} = 0,\ \forall \mathcal{J}_{\text{min}} \in \mathcal{S}_{\text{min}}^{\text{CPC}} \Longrightarrow \mathcal{J} = 0,\ \forall \mathcal{J} \in \mathcal{S}_{\text{gen}}/\mathcal{S}_{\text{min}}^{\text{CPC}}. \tag{3.23}$$

The most straightforward method to find such a minimal CPC set is to solve for the common zeros of polynomials in a candidate minimal CPC set,[12] and subsequently apply the solutions to the other CP-odd invariants to check whether they will vanish. However, this is not practical for complicated polynomials. Without directly solving the polynomial equations,

[11] By pseudo-real couplings, we denote a set of couplings which have irremovable phases but still conserve CP. This is the case in models with discrete symmetries, when the effect of a CP transformation on the Lagrangian parameters can be undone by a field redefinition, even if there exists no basis where all couplings can be made real. This has been previously noted in the context of Three Higgs Doublet Models [32] and toy models with more involved discrete symmetry groups [33].

[12] We have done this for the *generating* set of the νSM ($n_N = n_f = 2$) using the package `Macaulay2` [263], for which the complete set of CPC conditions are listed in App. 3.E. However, it is still difficult to obtain the common zeros of the subset of the generating invariants, thus we can not determine the minimal CPC set.

one can also use syzygies to determine whether other invariants are automatically zero given that all invariants in a minimal set are set to zero. This approach was e.g. followed in Ref. [250], where the author found some syzygies that can determine the minimal CPC set in the 2HDM. Here, we will show that a specific form of syzygy can help to determine whether an invariant will vanish.

The problem of finding the common zeros of polynomials is closely connected to Hilbert's Nullstellensatz [264–266], a theorem that establishes a fundamental relationship between geometry and algebra. We have presented this theorem and relevant mathematical terms in App. 3.D. In this section, we will employ Hilbert's Nullstellensatz to reframe the problem of identifying the minimal CPC set. We define an invariant ring, or more generally a polynomial ring $R := \mathbb{Q}[x_1, \dots, x_n]$, where $x_{1,\dots,n}$ are the parameters in the theory. The CP-odd generating invariants are polynomials in this ring, $\mathcal{J}_s, \mathcal{J}_1, \dots, \mathcal{J}_m \in R$. Hilbert's Nullstellensatz states that if an invariant $\mathcal{J}_s$ vanishes on all the common zeros of the $\mathcal{J}_{1,\dots,m}$, then there exist some integer t, such that $\mathcal{J}_s^t$ is a subset of the ideal $I := (\mathcal{J}_1, \dots, \mathcal{J}_m)$, i.e.,

$$\mathcal{J}_s^t = f_1 \mathcal{J}_1 + \cdots + f_m \mathcal{J}_m \,, \quad f_i \in R \,, \tag{3.24}$$

where f_i are the ring elements, i.e., they are polynomials of the parameters. However, since $\mathcal{J}_s$ and $\mathcal{J}_{1,\dots,m}$ are elements in the invariant ring, f_i should also be invariants. They can be parameterised by the generating invariants in a polynomial form

$$\mathcal{J}_s^t = \sum_{i=1}^{m} P_i(\mathcal{J}_l, \mathcal{I}_k) \mathcal{J}_i \,, \quad i \neq s \,. \tag{3.25}$$

Therefore, Hilbert's Nullstellensatz tells us that if a CP-odd invariant $\mathcal{J}_s$ is redundant in the presence of a given CPC set, there must exist a syzygy of some power of $\mathcal{J}_s$ that can be used to eliminate this invariant. For example, in Ref. [250] syzygies are used to identify the CPC conditions in the 2HDM. There, the syzygies of the type shown in Eq. (3.24) can be obtained at order $\mathcal{J}_s^2$ and there is no need to discuss the syzygies for different limits of the parameter spectrum as presented in their analysis.

It is possible to come up with an elimination algorithm based on the Hilbert's Nullstellensatz to find the minimal CPC set. However, the problem of finding a syzygy like Eq. (3.25), or in more mathematical language, determining whether an ideal $\mathcal{J}_s^t$ is a subset of another ideal $I := (\mathcal{J}_1, \dots, \mathcal{J}_m)$ highly relies on the calculation of the Gröbner basis, which is computationally quite expensive in complicated polynomial rings. The undetermined power t also introduces a lot of complexity in this problem. There are different methods and packages that are suitable for this problem. As outlined in Ref. [4], the syzygy problem can be converted to a finite system of linear equations, which can be addressed using standard linear algebra techniques. However, some high-degree syzygies lead to very complex linear systems that can not be easily solved. Some software systems are devoted to studying the algebraic geometry and commutative algebra, such as `Macaulay2` [263] and `Singular` [267]. In addition, there is the `Mathematica` function **PolynomialReduce**, which is however also based on the expensive determination of a Gröbner basis. Despite the capabilities of these packages, they failed to generate results within a reasonable time frame for the three-generation case of the νSM.

Although we were unable to construct the minimal CPC set for the theory with three generations of fermions, we did identify some example of syzygy that follows the form shown in Eq. (3.25). For instance,

$$\begin{aligned} 2\mathcal{J}_{14}^2 = \mathcal{J}_1\left(2\mathcal{J}_{34}\mathcal{I}_2 - 2\mathcal{J}_{76} - \mathcal{J}_{11}\mathcal{I}_2^2 - \mathcal{J}_{11}\mathcal{I}_5\right) + \mathcal{J}_3\left(4\mathcal{J}_{36} - 4\mathcal{J}_{13}\mathcal{I}_2 + \mathcal{I}_2^2\mathcal{J}_3 + \mathcal{I}_5\mathcal{J}_3\right) \\ + 2\mathcal{J}_4\left(\mathcal{J}_{11}\mathcal{I}_2 - \mathcal{J}_{34}\right) - 2\mathcal{J}_{11}\mathcal{J}_{15} + 2\mathcal{J}_{13}^2\,, \end{aligned} \tag{3.26}$$

one can find that if $\{\mathcal{J}_1, \mathcal{J}_3, \mathcal{J}_4, \mathcal{J}_{11}, \mathcal{J}_{13}\}$ is set to zero, then $\mathcal{J}_{14} = 0$ automatically, which means if we include the list of five invariants in the CPC set, the inclusion of $\mathcal{J}_{14}$ is no longer necessary.

In addition, we also find that some CP-odd invariants must be added to the minimal CPC set. Specifically, if only one CP-odd invariant $\mathcal{J}_s$ in the generating set is non-zero under a specific parameter spectrum, it necessarily has to be added to the minimal CPC set as it contains all ways of conserving CP in that theory. We have found 3 such cases where only one CP-odd invariant is non-zero. The first is the limit $M_N \to 0$ where the theory is reduced to a copy of the SM quark sector. Then the analogue of the Jarlskog invariant $\mathcal{J}_{10} = \operatorname{Im}\operatorname{Tr}\left(X_N^2 X_e^2 X_N X_e\right)$ is the only non-vanishing CP-odd invariant and has to be included in the minimal CPC set. The other 2 cases are found under the spectrum $\{M_N \to m_N \mathbb{1}, Y_e \to 0\}$ and $\{M_N \to m_N \mathbb{1}, Y_N \to y_N \mathbb{1}\}$ which force us to add $\mathcal{J}_{74} = \operatorname{Im}\operatorname{Tr}\left(Y_N Y_N^\dagger Y_N M_N^* Y_N^T Y_N^* M_N Y_N^\dagger Y_N M_N^* Y_N^T Y_N^* Y_N^T Y_N^* M_N Y_N^\dagger\right)$ and $\mathcal{J}_{251} = \operatorname{Im}\operatorname{Tr}\left(X_e^2 Y_N M_N^* Y_N^T X_e^{*2} Y_N^* M_N Y_N^\dagger X_e Y_N M_N^* Y_N^T X_e^* Y_N^* M_N Y_N^\dagger\right)$ to the minimal CPC set respectively. It is interesting that we have to rely on the highest-order invariant $\mathcal{J}_{251}$ to establish the CPC conditions of the theory (c.f. the full invariant list in Ref. [4]).

We want to emphasise one point here. The parameters of the neutrino sector are not measured well enough today to even exclude that one of the neutrinos is massless. Therefore, having a set of flavour invariants which determines the CPC conditions without assumptions on the spectrum is important to make general statements about the theory that hold true for all possible experimental results.

Appendices to Chapter 3

3.A Parameterisation of Flavour Matrices

3.A.1 Standard Parameterisation

The parameterisations of the flavour matrices in the lepton and quark sectors have been discussed in detail in Refs. [218, 261]. Because we use slightly different conventions here, we will discuss the reduction of the flavour matrices to a minimal parameterisation here. The fermionic part of the Lagrangian is given by

$$\mathcal{L}_4 \supset \sum_{\Psi} \bar{\Psi} i \not{D} \Psi - \left[\frac{1}{2} \left(N C M_N N \right) + \bar{L} Y_N N \widetilde{H} + \bar{L} Y_e e H + \bar{Q} Y_u u \widetilde{H} + \bar{Q} Y_d d H + \text{H.c.} \right], \tag{3.27}$$

where the kinetic term sums all fermion fields $\Psi = \{Q, L, u, d, e, N\}$. Performing a single value decomposition on the matrices we have

$$\begin{aligned} Y_e &= V_e \, \widehat{Y}_e \, W_e^{\dagger} \,, \quad Y_N = V_N \, \widehat{Y}_N \, W_N^{\dagger} \,, \quad M_N = V_N' \, \widehat{M}_N \, V_N'^T \,, \\ Y_u &= V_u \, \widehat{Y}_u \, W_u^{\dagger} \,, \quad Y_d = V_d \, \widehat{Y}_d \, W_d^{\dagger} \,, \end{aligned} \tag{3.28}$$

where $\widehat{Y}_{N,e,u,d}$ and $\widehat{M}_N$ are diagonal matrices with real and non-negative entries. V_f, W_f with $f = N, e, u, d$ and V_N' are unitary matrices. Using appropriate flavour transformation on the gauge fields most of this matrices can be removed and we can reduce the matrices to the following form

$$\begin{aligned} Y_e &= \widehat{Y}_e \,, \quad Y_N = V_L \, \widehat{Y}_N \, W^{\dagger} \,, \quad M_N = \widehat{M}_N \,, \\ Y_u &= \widehat{Y}_u \,, \quad Y_d = V_{\text{CKM}} \, \widehat{Y}_d \,, \end{aligned} \tag{3.29}$$

where $V_{\text{CKM}} = V_u^{\dagger} V_d$ is the CKM matrix, describing the misalignment of the up- and down-type quark mass basis. $V_L = V_e^{\dagger} V_N$ in the lepton sector arises in the same way and describes the misalignment between the lepton Yukawa matrices. The existence of the Majorana mass matrix in the lepton sector introduces another mixing matrix $W = V_N'^T W_N$, which describes the mismatch between the diagonalisation matrices of Y_N and M_N. For a lepton number-conserving Dirac neutrino mass, M_N is set to zero and only the mixing matrix V_L will be present in the theory, which can be directly identified with the PMNS matrix, which in this case has the same form as the CKM matrix without any additional phases.

From Eq. (3.28), by assuming that the flavour matrices have no degenerate or vanishing eigenvalues,[13] the diagonalisation matrices will at least have a column phase redefinition freedom, $V_f \to V_f e^{i\widehat{\Phi}_f}$, $W_f \to W_f e^{i\widehat{\Phi}_f}$, $f = \{N, e, u, d\}$ and $V_N' \to V_N' \eta_N$. Applied to Eq. (3.29)

[13] If there are degenerate or vanishing masses, the exact flavour group of the renormalisable Lagrangian might increase. In that case, more parameters can be absorbed by performing field redefinitions rendering these parameters unphysical. Ideally, these parameters should always be removed in the parameterisation, such that the most minimal parameterisation is used in practice.

this implies

$$e^{i\widehat{\Phi}_f}\widehat{Y}_f e^{-i\widehat{\Phi}_f} = \widehat{Y}_f, \quad \eta_N \widehat{M}_N \eta_N = \widehat{M}_N\,, \tag{3.30}$$

where $\widehat{\Phi}_f \equiv \mathrm{diag}(\phi_{f1}, \phi_{f2}, \phi_{f3})\,, f = N, e, u, d$ are diagonal matrices of phases, and η_N is a diagonal matrix with eigenvalues ±1. Under these rephasings, the mixing matrices transform as

$$V_{\mathrm{CKM}} \to e^{-i\widehat{\Phi}_u} V_{\mathrm{CKM}} e^{i\widehat{\Phi}_d}\,, \quad V_L \to e^{-i\widehat{\Phi}_e} V_L e^{i\widehat{\Phi}_N}\,, \quad W \to \eta_N W e^{i\widehat{\Phi}_N}\,, \tag{3.31}$$

Then, the 3×3 unitary matrix can be parameterised as

$$U_3 = e^{i\varphi} e^{i\widehat{\Psi}} U(\theta_{12}, \theta_{13}, \theta_{22}, \delta) e^{i\widehat{\Phi}}\,, \tag{3.32}$$

where φ is an overall phase, $\widehat{\Psi} = \mathrm{diag}(0, \psi_1, \psi_2)$ and $\widehat{\Phi} = \mathrm{diag}(0, \phi_1, \phi_2)$, and $U(\theta_{12}, \theta_{13}, \theta_{23}, \delta)$ takes the standard form

$$U(\theta_{12}, \theta_{13}, \theta_{23}, \delta) \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta} \\ 0 & 1 & 0 \\ -s_{13}e^{i\delta} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.33}$$

where $s_{ij} \equiv \sin\theta_{ij}$, $c_{ij} \equiv \cos\theta_{ij}$, and $\theta_{ij} \in [0, \pi/2], \delta \in [0, 2\pi)$.

Due to the rephasings in Eq. (3.31), the additional phases in the unitary matrix V_{CKM} can be absorbed, and it will take the form introduced in Eq. (2.3). The quark sector has the following number of parameters

Matrices	Masses	Angles	Phases
$\widehat{Y}_u$	3	0	0
$\widehat{Y}_d$	3	0	0
V_{CKM}	0	3	1
Total	6	3	1

There are a total of 10 parameters, consisting of 6 quark masses, 3 mixing angles, and 1 phase.

In the lepton sector, the mixing matrices can be parameterised as follows

$$\begin{aligned} V_L &= e^{i\varphi} e^{i\widehat{\Psi}} U(\theta_{12}, \theta_{13}, \theta_{23}, \delta) e^{i\widehat{\Phi}}\,, \\ W &= e^{i\varphi'} e^{i\widehat{\Psi}'/2} U(\theta'_{12}, \theta'_{13}, \theta'_{23}, \delta') e^{i\widehat{\Phi}'}\,. \end{aligned} \tag{3.34}$$

Since V_L and W share the same rephasing matrix $\widehat{\Phi}_N$, we can use this freedom to remove either $\widehat{\Phi}$ or $\widehat{\Phi}'$ in Eq. (3.34) at will. Using the rephasings $\widehat{\Phi}_e$ and $\widehat{\Phi}_N$ to remove the phases in V_L and the phase φ' in W in Eq. (3.34), without loss of generality, the mixing matrices take the following form

$$V_L = U(\theta_{12}, \theta_{13}, \theta_{23}, \delta)\,, \quad W = e^{i\widehat{\Psi}'/2} U(\theta'_{12}, \theta'_{13}, \theta'_{23}, \delta') e^{i\widehat{\Phi}'}\,. \tag{3.35}$$

Instead, we could also move one of the phase matrices to V_L

$$V_L = U(\theta_{12}, \theta_{13}, \theta_{23}, \delta) e^{i\widehat{\Phi}}\,, \quad W = e^{i\widehat{\Psi}'/2} U(\theta'_{12}, \theta'_{13}, \theta'_{23}, \delta')\,. \tag{3.36}$$

This corresponds to the most general parameterisation of the mixing matrices V_L and W and we will work in this basis without loss of generality. To be specific, we use the following parameterisation of the flavour matrices

$$Y_e = \mathrm{diag}\,(y_e, y_\mu, y_\tau)\,,\; Y_N = V_L \cdot \mathrm{diag}\,(y_1, y_2, y_3) \cdot W^\dagger,\; M_N = \mathrm{diag}\,(m_1, m_2, m_3)\,, \tag{3.37}$$

with V_L and W defined in Eq. (3.36). We summarise the number of parameters in each matrix in Tab. 3.4.

For a more comprehensive discussion, we refer to Ref. [218]. There, also the cases $n_N = n_f = 2$ and $n_N = 2, n_f = 3$ in the lepton sector are discussed. For $n_N = n_f = 2$, all flavour matrices are 2×2 matrices and they can be parameterised as follows following a similar discussion

$$Y_e = \mathrm{diag}\,(y_e, y_\mu)\,, \qquad Y_N = V_L \cdot \mathrm{diag}\,(y_1, y_2) \cdot W^\dagger, \qquad M_N = \mathrm{diag}\,(m_1, m_2)\,, \tag{3.38}$$

with

$$V_L = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \cdot \mathrm{diag}\left(1, e^{i\phi}\right), \quad W = \mathrm{diag}\left(1, e^{i\varphi}\right) \cdot \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}. \tag{3.39}$$

For $n_N = 2, n_f = 3$, Y_N is a 3×2 matrix, and M_N is a 2×2 matrix. Then, the flavour matrices can be parameterised as

$$Y_e = \mathrm{diag}\,(y_e, y_\mu, y_\tau)\,, \quad Y_N = V_L \cdot \begin{pmatrix} y_1 & 0 \\ 0 & y_2 \\ 0 & 0 \end{pmatrix} \cdot W^\dagger, \quad M_N = \mathrm{diag}\,(m_1, m_2)\,, \tag{3.40}$$

where V_L and W are given by

$$V_L = U(\theta_{12}, \theta_{13}, \theta_{23}, \delta) \cdot \mathrm{diag}\left(1, e^{i\phi}, 1\right), \quad W = \mathrm{diag}\left(1, e^{i\varphi}\right) \cdot \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}, \tag{3.41}$$

in analogy to the parameterisation in Eq. (3.36), where the last phase in $\hat{\Phi}$ is unphysical, because it is multiplied by zeros in $\hat{Y}_N$.

Matrices	Masses	Angles	Phases
$\widehat{M}_N$	3 [2] (2)	0	0
$\widehat{Y}_N$	3 [2] (2)	0	0
$\widehat{Y}_e$	3 [2] (3)	0	0
V_L	0	3 [1] (3)	3 [1] (2)
W	0	3 [1] (1)	3 [1] (1)
Total	9 [6] (7)	6 [2] (4)	6 [2] (3)

Table 3.4: The number of masses, mixing angles and phases in the parameterisation of the lepton sector for the case of $n_N = n_f = 3\,[n_N = n_f = 2]\,(n_N = 2, n_f = 3)$.

In the Dirac limit, M_N is set to zero, and we can simply set $W = \mathbb{1}$. In the case of $n_N = n_f = 3$, the matrix V_L will become the PMNS matrix V_{PMNS}, which takes the same standard form as V_{CKM}. The parameterisation is given as

$$Y_e = \text{diag}\,(y_e, y_\mu, y_\tau)\,, \quad Y_N = U(\theta_{12}, \theta_{13}, \theta_{23}, \delta) \cdot \text{diag}\,(y_1, y_2, y_3)\,. \tag{3.42}$$

Similarly, for $n_N = n_f = 2$, it can be parameterised as

$$Y_e = \text{diag}\,(y_e, y_\mu)\,, \qquad Y_N = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \cdot \text{diag}\,(y_1, y_2)\,, \tag{3.43}$$

where the phase of V_L in the Majorana case can be removed by the rephasing of the right-handed neutrino N. For $n_N = 2, n_f = 3$, the parameterisation is given by

$$Y_e = \text{diag}\,(y_e, y_\mu, y_\tau)\,, \quad Y_N = U(\theta_{12}, \theta_{13}, \theta_{23}, \delta) \cdot \begin{pmatrix} y_1 & 0 \\ 0 & y_2 \\ 0 & 0 \end{pmatrix}, \tag{3.44}$$

where the phase $e^{i\phi}$ in Eq. (3.41) can be absorbed by the field N in the Dirac case. The parameters in the Dirac limit are summarised in Tab. 3.5.

3.A.2 Algebraic Parameterisation

The parameterisation described above is favoured for its phenomenological relevance, as Yukawa matrices are factorised into eigenvalues and mixing matrices, which aligns with experimental observables. However, when exploring the algebraic structures of invariants, the inclusion of trigonometric functions introduces complexity. The use of sine and cosine as ob-

Matrices	Masses	Angles	Phases
$\widehat{Y}_N$	3[2](2)	0	0
$\widehat{Y}_e$	3[2](3)	0	0
V_{PMNS}	0	3[1](3)	1[0](1)
Total	6[4](5)	3[1](3)	1[0](1)

Table 3.5: The number of masses, mixing angles and phases in the parameterisation of the lepton sector for the case of $n_N = n_f = 3\,[n_N = n_f = 2]\,(n_N = 2, n_f = 3)$ in the Dirac limit.

jects in the polynomial expansion of flavour invariants can complicate the exploration of these structures. Consequently, alternative parameterisations that are more suitable for polynomial expressions are needed.

One possible solution is to parameterise the trigonometric functions. A frequently used parameterisation for the unit circle is

$$x(t) = \frac{1-t^2}{1+t^2}, \quad y(t) = \frac{2t}{1+t^2}, \quad \text{with } t \in (-\infty, +\infty). \tag{3.45}$$

However the point $(-1,0)$ on the unit circle can only be obtained in the limit $t \to \infty$. Another parameterisation that can cover the whole circle is given by

$$x(t) = \frac{1-6t^2+t^4}{1+2t^2+t^4}, \quad y(t) = \frac{4t-4t^3}{1+2t^2+t^4}, \quad \text{with } t \in (-1,1]\,. \tag{3.46}$$

Thus the sine and cosine functions in the mixing matrices of our above parameterisation can be replaced with $x(t)$ and $y(t)$ respectively. However, this parameterisation may introduce new complexities, as it leads to rational polynomials.

Following the parameterisation in Eq. (3.37), it is possible to work with the diagonal basis of both Y_e and M_N while leaving Y_N undiagonalised

$$Y_e = \text{diag}\,(y_e, y_\mu, y_\tau)\,, \quad Y_N = \begin{pmatrix} r_{11} & c_{12} & c_{13} \\ r_{21} & c_{22} & c_{23} \\ r_{31} & c_{32} & c_{33} \end{pmatrix}, \quad M_N = \text{diag}\,(m_1, m_2, m_3)\,, \tag{3.47}$$

where r_{ij} and c_{ij} are general labels for real and complex parameters respectively. The phases of the first column of Y_N are absorbed by the rephasing of the charged lepton fields.[14] In this parameterisation all invariants are expressed as polynomials of simple variables, making it easier to analyze the algebraic structures of the theory. It is easy to see that the number

[14]It is not necessary for the rephasing degree of freedom to target the first column, any phase in each row of Y_N can be eliminated.

of parameters in this parameterisation is still 21, which is the same as the physical parameterisation in Eq. (3.37). Similarly, for $n_N = n_f = 2$, we can parameterise the flavour matrices as

$$Y_e = \mathrm{diag}\left(y_e, y_\mu\right), \qquad Y_N = \begin{pmatrix} r_{11} & c_{12} \\ r_{21} & c_{22} \end{pmatrix}, \qquad M_N = \mathrm{diag}\left(m_1, m_2\right). \tag{3.48}$$

For $n_N = 2, n_f = 3$, the parameterisation is given by

$$Y_e = \mathrm{diag}\left(y_e, y_\mu, y_\tau\right), \quad Y_N = \begin{pmatrix} r_{11} & c_{12} \\ r_{21} & c_{22} \\ r_{31} & c_{32} \end{pmatrix}, \quad M_N = \mathrm{diag}\left(m_1, m_2\right). \tag{3.49}$$

The mapping between these two parameterisations can be found by solving equations built from the entries of Y_N, which will not be shown here.

In the Dirac limit where the Majorana mass term M_N is set to 0, the parameters in Yukawa matrix Y_N can be further reduced by the field redefinition of right-handed neutrino N, which is explained in detail in Ref. [4]. We find

$$Y_e = \mathrm{diag}\left(y_e, y_\mu, y_\tau\right), \quad Y_N = \begin{pmatrix} r_{11} & 0 & 0 \\ r_{21} & r_{22} & 0 \\ r_{31} & c_{32} & r_{33} \end{pmatrix}. \tag{3.50}$$

We find there are exactly 10 real parameters in this parameterisation, as expected. Similarly, for $n_N = n_f = 2$ the flavour matrices are parameterised as

$$Y_e = \mathrm{diag}\left(y_e, y_\mu\right), \qquad Y_N = \begin{pmatrix} r_{11} & 0 \\ r_{21} & r_{22} \end{pmatrix}. \tag{3.51}$$

For $n_N = 2, n_f = 3$ the parameterisation is given by

$$Y_e = \mathrm{diag}\left(y_e, y_\mu, y_\tau\right), \quad Y_N = \begin{pmatrix} r_{11} & 0 \\ r_{21} & r_{22} \\ r_{31} & c_{32} \end{pmatrix}. \tag{3.52}$$

3.B Results for Multi-Graded Hilbert Series and Plethystic Logarithm

3.B.1 Model with $n_N = n_f = 3$

In Eqs. (3.6) and (3.7), we have presented the ungraded Hilbert series, where the same grading is used for all spurions. However, the information encoded in the ungraded Hilbert series is not enough for analyses, where the plethystic logarithm is used to count the number of generating invariants and syzygies at each order. Therefore, in this section, we present the multi-graded Hilbert series, where the single spurion q in Eqs. (3.6) and (3.7) is traded for multiple spurions e, m and n, corresponding to the spurions of the flavour matrices Y_e, M_N and Y_N respectively. The denominator of the multi-graded Hilbert series is given as follows

$$\begin{aligned}\mathcal{D}(e,m,n) = &(1-e^2)(1-m^2)(1-n^2)(1-e^4)(1-m^4)(1-n^4)(1-e^2n^2)^2(1-m^2n^2)\\&(1-e^6)(1-m^6)(1-n^6)(1-e^2n^4)(1-e^4n^2)(1-m^2n^4)^2(1-m^4n^2)(1-e^2m^2n^2)\\&(1-m^2n^6)(1-m^4n^4)(1-e^2m^2n^4)(1-e^2m^4n^2)(1-e^4m^2n^2)(1-m^2n^8)\\&(1-e^2m^2n^6)(1-e^4m^2n^4)(1-e^4m^4n^2)(1-e^4m^2n^6)(1-e^4m^4n^4)(1-e^6m^2n^4)\\&(1-e^4m^2n^8)(1-e^8m^2n^4)(1-e^8m^4n^4)\,,\end{aligned} \tag{3.53}$$

while there are 6582 terms in the numerator, which goes up to order $\mathcal{O}([emn]^{196})$ in total powers of spurions. Due to its length we only show the terms up to $\mathcal{O}([emn]^{26})$ below

$$\begin{aligned}\mathcal{N}(e,m,n) = &1-e^2n^2+2m^4n^4+e^4n^4+2e^2m^2n^4+2m^4n^6+2m^6n^4+4e^2m^2n^6\\&+4e^2m^4n^4+3e^4m^2n^4+3m^4n^8+3m^6n^6+m^8n^4+5e^2m^2n^8+7e^2m^4n^6+3e^2m^6n^4\\&+4e^4m^2n^6+5e^4m^4n^4+e^6m^2n^4+m^4n^{10}+3m^6n^8+m^8n^6+3e^2m^2n^{10}+9e^2m^4n^8\\&+6e^2m^6n^6+e^2m^8n^4+4e^4m^2n^8+10e^4m^4n^6+5e^4m^6n^4+3e^6m^2n^6+3e^6m^4n^4\\&+m^4n^{12}+m^6n^{10}+3m^8n^8+e^2m^2n^{12}+5e^2m^4n^{10}+9e^2m^6n^8+2e^2m^8n^6+e^4m^2n^{10}\\&+16e^4m^4n^8+10e^4m^6n^6+2e^4m^8n^4+4e^6m^2n^8+8e^6m^4n^6+3e^6m^6n^4+2e^8m^2n^6\\&+e^8m^4n^4+m^8n^{10}+m^{10}n^8+e^2m^4n^{12}+6e^2m^6n^{10}+7e^2m^8n^8-e^2m^{10}n^6\\&+10e^4m^4n^{10}+19e^4m^6n^8+4e^4m^8n^6+e^6m^2n^{10}+14e^6m^4n^8+8e^6m^6n^6+e^6m^8n^4\\&+e^8m^2n^8+5e^8m^4n^6+2e^8m^6n^4+e^{10}m^2n^6-m^6n^{14}+2m^{10}n^{10}+m^{12}n^8-3e^2m^4n^{14}\\&+2e^2m^6n^{12}+5e^2m^8n^{10}+2e^2m^{10}n^8-e^2m^{12}n^6-e^4m^2n^{14}+6e^4m^4n^{12}+15e^4m^6n^{10}\\&+12e^4m^8n^8-2e^4m^{10}n^6-e^6m^2n^{12}+9e^6m^4n^{10}+16e^6m^6n^8+2e^6m^8n^6-2e^8m^2n^{10}\\&+9e^8m^4n^8+4e^8m^6n^6+e^8m^8n^4-2e^{10}m^2n^8+2e^{10}m^4n^6-m^6n^{16}-2m^8n^{14}+m^{12}n^{10}\\&-2e^2m^4n^{16}-4e^2m^6n^{14}+3e^2m^8n^{12}+2e^2m^{10}n^{10}-2e^4m^4n^{14}+6e^4m^6n^{12}+7e^4m^8n^{10}\\&-e^4m^{10}n^8-2e^4m^{12}n^6-2e^6m^2n^{14}+2e^6m^4n^{12}+13e^6m^6n^{10}+8e^6m^8n^8-3e^6m^{10}n^6\\&-3e^8m^2n^{12}+3e^8m^4n^{10}+8e^8m^6n^8+2e^8m^8n^6-2e^{10}m^2n^{10}-3e^{10}m^4n^8-e^{12}m^2n^8\\&-m^8n^{16}-m^{10}n^{14}-e^2m^4n^{18}-3e^2m^6n^{16}-6e^2m^8n^{14}-e^2m^{10}n^{12}-3e^2m^{12}n^{10}\\&+e^4m^4n^{16}-10e^4m^6n^{14}-5e^4m^8n^{12}-7e^4m^{10}n^{10}-3e^4m^{12}n^8-7e^6m^4n^{14}+2e^6m^6n^{12}\\&-e^6m^8n^{10}-2e^6m^{10}n^8-2e^6m^{12}n^6-2e^8m^2n^{14}-4e^8m^4n^{12}+2e^8m^6n^{10}+3e^8m^8n^8\\&-2e^8m^{10}n^6-2e^{10}m^2n^{12}-6e^{10}m^4n^{10}-3e^{10}m^6n^8-3e^{12}m^4n^8-3m^{10}n^{16}-m^{12}n^{14}\\&-m^{14}n^{12}-e^2m^6n^{18}-7e^2m^8n^{16}-10e^2m^{10}n^{14}-5e^2m^{12}n^{12}-2e^2m^{14}n^{10}-15e^4m^6n^{16}\\&-33e^4m^8n^{14}-22e^4m^{10}n^{12}-13e^4m^{12}n^{10}-e^4m^{14}n^8-2e^6m^4n^{16}-21e^6m^6n^{14}\\&-21e^6m^8n^{12}-16e^6m^{10}n^{10}-4e^6m^{12}n^8-11e^8m^4n^{14}-15e^8m^6n^{12}-15e^8m^8n^{10}\\&-6e^8m^{10}n^8-2e^8m^{12}n^6-e^{10}m^2n^{14}-9e^{10}m^4n^{12}-8e^{10}m^6n^{10}-5e^{10}m^8n^8-e^{10}m^{10}n^6\\&-3e^{12}m^6n^8-e^{14}m^4n^8+\mathcal{O}([emn]^{28})\,.\end{aligned} \tag{3.54}$$

It is worth noting that the multi-graded Hilbert series lacks certain properties of the ungraded Hilbert series, such as a matching number of factors in the denominator with physical observables and a palindromic form in the numerator. As already mentioned in footnote 5, there is an ambiguity when determining the form of the ungraded Hilbert series, which makes the plethystic logarithm more helpful in our case, since it is unique for both the ungraded and multi-graded Hilbert series.

The invariants in our theory form a non-complete intersection ring making the plethystic logarithm a non-terminating series as a result. According to Eq. (2.94), the plethystic logarithm can only be calculated up to some given order in the spurions. However, as we discussed in Sec. 3.2.2, we are only interested in the terms in the plethystic logarithm up to the first purely negative order, which we find to occur at order $\mathcal{O}([emn]^{26})$. The plethystic logarithm up to this order is given by

$$\begin{aligned}
\mathrm{PL}(e,m,n) = &\left(e^2+m^2+n^2\right)+\left(e^4+m^4+n^4+e^2n^2+m^2n^2\right)+\left(e^6+m^6+n^6+e^2n^4\right.\\
&\left.+e^4n^2+2m^2n^4+m^4n^2+e^2m^2n^2\right)+\left(e^4n^4+m^2n^6+3m^4n^4+3e^2m^2n^4+e^2m^4n^2\right.\\
&\left.+e^4m^2n^2\right)+\left(m^2n^8+2m^4n^6+2m^6n^4+5e^2m^2n^6+4e^2m^4n^4+4e^4m^2n^4+e^4m^4n^2\right)\\
&+\left(e^6n^6+3m^4n^8+3m^6n^6+m^8n^4+5e^2m^2n^8+9e^2m^4n^6+3e^2m^6n^4+7e^4m^2n^6\right.\\
&\left.+6e^4m^4n^4+2e^6m^2n^4\right)+\left(m^4n^{10}+3m^6n^8+m^8n^6+3e^2m^2n^{10}+11e^2m^4n^8\right.\\
&+8e^2m^6n^6+e^2m^8n^4+9e^4m^2n^8+14e^4m^4n^6+5e^4m^6n^4+6e^6m^2n^6+3e^6m^4n^4\\
&\left.+e^8m^2n^4\right)+\left(m^4n^{12}+m^6n^{10}+e^2m^2n^{12}+8e^2m^4n^{10}+8e^2m^6n^8+3e^2m^8n^6\right.\\
&+6e^4m^2n^{10}+20e^4m^4n^8+13e^4m^6n^6+2e^4m^8n^4+8e^6m^2n^8+13e^6m^4n^6\\
&\left.+3e^6m^6n^4+3e^8m^2n^6+2e^8m^4n^4\right)+\left(2e^2m^4n^{12}+3e^4m^2n^{12}+11e^4m^4n^{10}\right.\\
&+11e^4m^6n^8+5e^4m^8n^6+5e^6m^2n^{10}+18e^6m^4n^8+13e^6m^6n^6+e^6m^8n^4+4e^8m^2n^8\\
&+8e^8m^4n^6+2e^8m^6n^4+e^{10}m^2n^6-3m^8n^{10}-3m^{10}n^8-3e^2m^6n^{10}-4e^2m^8n^8\\
&\left.-e^2m^{10}n^6\right)+\left(2e^6m^6n^8+4e^6m^8n^6+9e^8m^4n^8+7e^8m^6n^6+e^8m^8n^4+3e^{10}m^4n^6\right.\\
&-m^6n^{14}-9m^8n^{12}-8m^{10}n^{10}-4m^{12}n^8-2e^2m^4n^{14}-21e^2m^6n^{12}-32e^2m^8n^{10}\\
&-14e^2m^{10}n^8-e^2m^{12}n^6-9e^4m^4n^{12}-28e^4m^6n^{10}-18e^4m^8n^8-2e^4m^{10}n^6\\
&\left.-e^6m^4n^{10}\right)+\left(3e^8m^8n^6+2e^{10}m^6n^6-m^6n^{16}-10m^8n^{14}-18m^{10}n^{12}-9m^{12}n^{10}\right.\\
&-2m^{14}n^8-2e^2m^4n^{16}-34e^2m^6n^{14}-76e^2m^8n^{12}-55e^2m^{10}n^{10}-12e^2m^{12}n^8\\
&-27e^4m^4n^{14}-103e^4m^6n^{12}-109e^4m^8n^{10}-39e^4m^{10}n^8-2e^4m^{12}n^6-2e^6m^2n^{14}\\
&-45e^6m^4n^{12}-83e^6m^6n^{10}-35e^6m^8n^8-3e^6m^{10}n^6-6e^8m^2n^{12}-21e^8m^4n^{10}\\
&\left.-9e^8m^6n^8-4e^{10}m^2n^{10}-e^{10}m^4n^8\right)+\left(e^{10}m^8n^6-e^{12}n^{12}-11m^8n^{16}-20m^{10}n^{14}\right.\\
&-21m^{12}n^{12}-5m^{14}n^{10}-m^{16}n^8-e^2m^4n^{18}-33e^2m^6n^{16}-110e^2m^8n^{14}-116e^2m^{10}n^{12}\\
&-48e^2m^{12}n^{10}-5e^2m^{14}n^8-31e^4m^4n^{16}-174e^4m^6n^{14}-284e^4m^8n^{12}-162e^4m^{10}n^{10}\\
&-33e^4m^{12}n^8-e^6m^2n^{16}-87e^6m^4n^{14}-261e^6m^6n^{12}-226e^6m^8n^{10}-59e^6m^{10}n^8\\
&-2e^6m^{12}n^6-8e^8m^2n^{14}-94e^8m^4n^{12}-134e^8m^6n^{10}-48e^8m^8n^8-2e^8m^{10}n^6\\
&\left.-10e^{10}m^2n^{12}-32e^{10}m^4n^{10}-15e^{10}m^6n^8-3e^{12}m^2n^{10}-2e^{12}m^4n^8\right)+\left(-5m^8n^{18}\right.\\
&-19m^{10}n^{16}-16m^{12}n^{14}-7m^{14}n^{12}-m^{16}n^{10}-22e^2m^6n^{18}-105e^2m^8n^{16}
\end{aligned} \tag{3.55}$$

$$
\begin{aligned}
&-149e^2m^{10}n^{14} - 88e^2m^{12}n^{12} - 20e^2m^{14}n^{10} - e^2m^{16}n^8 - 21e^4m^4n^{18} - 192e^4m^6n^{16} \\
&-424e^4m^8n^{14} - 371e^4m^{10}n^{12} - 130e^4m^{12}n^{10} - 13e^4m^{14}n^8 - 96e^6m^4n^{16} - 448e^6m^6n^{14} \\
&-603e^6m^8n^{12} - 303e^6m^{10}n^{10} - 45e^6m^{12}n^8 - 5e^8m^2n^{16} - 161e^8m^4n^{14} - 417e^8m^6n^{12} \\
&-314e^8m^8n^{10} - 70e^8m^{10}n^8 - 2e^8m^{12}n^6 - 12e^{10}m^2n^{14} - 108e^{10}m^4n^{12} - 140e^{10}m^6n^{10} \\
&-40e^{10}m^8n^8 - e^{10}m^{10}n^6 - 8e^{12}m^2n^{12} - 23e^{12}m^4n^{10} - 9e^{12}m^6n^8 - e^{14}m^2n^{10} - e^{14}m^4n^8\big) \\
&+\mathcal{O}\left([emn]^{28}\right) ,
\end{aligned}
$$

where the terms are grouped by parentheses at each order. We can see that the terms in $\mathcal{O}([emn]^{26})$ are all negative.

Under the Dirac limit, the Hilbert series can be obtained by setting $m \to 0$, which will have a very simple form as has been found for the quark sector in Eq. (2.96) after setting $e \to 0, u \to n, d \to e$

$$
\begin{aligned}
\mathcal{H}(e,n) &= \left(1 + e^6n^6\right) \times \qquad (3.56)\\
&\times \frac{1}{(1-e^2)(1-e^4)(1-e^6)(1-n^2)(1-n^4)(1-n^6)(1-e^2n^2)(1-e^4n^2)(1-e^2n^4)(1-e^4n^4)} .
\end{aligned}
$$

The ungraded Hilbert series is given by

$$
\mathcal{H}(q) = \frac{1+q^{12}}{(1-q^2)^2(1-q^4)^3(1-q^6)^4(1-q^8)} . \qquad (3.57)
$$

The Dirac case corresponds to a complete intersection ring, and the multi-graded plethystic logarithm has finite number of terms, which are given as follows

$$
\mathrm{PL}(e,n) = e^2 + e^4 + e^6 + n^2 + n^4 + n^6 + e^2n^2 + e^4n^2 + e^2n^4 + e^4n^4 + e^6n^6 - e^{12}n^{12} . \qquad (3.58)
$$

The corresponding ungraded plethystic logarithm can be obtained by setting $e, n \to q$, which has the following form

$$
\mathrm{PL}(q) = 2q^2 + 3q^4 + 4q^6 + q^8 + q^{12} - q^{24} , \qquad (3.59)
$$

where the positive terms correctly capture the 10 CP-even and 1 CP-odd invariants, while the negative term indicates there is a syzygy at order 24.

3.B.2 Model with $n_N = n_f = 2$

For completeness, we also show the Hilbert series for the case $n_N = n_f = 2$, which has already been presented in Ref. [218]. The numerator and denominator are given by

$$
\begin{aligned}
\mathcal{N}(e,m,n) =& 1 + 2e^2m^2n^4 + m^4n^4 + e^2m^4n^4 + e^4m^4n^4 + e^2m^2n^6 + e^4m^2n^6 - e^2m^6n^6 + \\
& - e^4m^6n^6 - e^2m^4n^8 - e^4m^4n^8 - e^6m^4n^8 - 2e^4m^6n^8 - e^6m^8n^{12} , \\
\mathcal{D}(e,m,n) =& \left(1-e^2\right)\left(1-e^4\right)\left(1-m^2\right)\left(1-m^4\right)\left(1-n^2\right)\left(1-e^2n^2\right)\left(1-m^2n^2\right) \times \\
& \left(1-e^2m^2n^2\right)\left(1-n^4\right)\left(1-m^2n^4\right)\left(1-e^4m^2n^4\right) .
\end{aligned}
\qquad (3.60)
$$

The ungraded Hilbert series is

$$\mathcal{H}(q) = \frac{1 + q^6 + 3q^8 + 2q^{10} + 3q^{12} + q^{14} + q^{20}}{(1-q^2)^3\,(1-q^4)^5\,(1-q^6)\,(1-q^{10})}\,. \tag{3.61}$$

The multi-graded plethystic logarithm is given by

$$\begin{aligned}\mathrm{PL}(e,m,n) =& e^2 + m^2 + n^2 + e^4 + m^4 + e^2n^2 + m^2n^2 + n^4 + e^2m^2n^2 + m^2n^4 + \\ &+ 2e^2m^2n^4 + m^4n^4 + e^4m^2n^4 + e^2m^4n^4 + e^2m^2n^6 + e^4m^4n^4 + \\ &+ e^4m^2n^6 - e^2m^6n^6 - e^2m^4n^8 - \mathcal{O}([emn]^{16})\,.\end{aligned} \tag{3.62}$$

As before, the plethystic logarithm is also a non-terminating series for two generations. Therefore, the theory corresponds to a non-complete intersection ring. However, the pure negative order appears already at $\mathcal{O}([emn]^{14})$, the 18 lower order terms in plethystic logarithm are all positive, and they correspond to the *generating* set presented in Eq. (3.66).

3.B.3 Model with $n_N = 2,\ n_f = 3$

For the case of $n_N = 2, n_f = 3$, the Hilbert series has been calculated in Ref. [252]. For completeness, we also provide it here. The numerator and denominator of the multi-graded Hilbert series are given by

$$\begin{aligned}\mathcal{N}(e,m,n) =& 1 - e^2n^2 + e^4n^4 + 2e^2m^2n^4 + 2e^4m^2n^4 + 2e^6m^2n^4 + m^4n^4 + e^2m^4n^4 + 2e^4m^4n^4 + \\ &+ e^6m^4n^4 + e^8m^4n^4 + e^2m^2n^6 + e^{10}m^2n^6 - e^2m^4n^6 - e^4m^4n^6 - 3e^6m^4n^6 + \\ &- e^8m^4n^6 - e^{10}m^4n^6 - e^2m^6n^6 - 2e^4m^6n^6 - 2e^6m^6n^6 - 2e^8m^6n^6 - e^{10}m^6n^6 + \\ &- e^4m^2n^8 - e^6m^2n^8 - e^8m^2n^8 - e^{10}m^2n^8 - e^{12}m^2n^8 - e^2m^4n^8 - e^4m^4n^8 + \\ &- 3e^6m^4n^8 - e^8m^4n^8 - 3e^{10}m^4n^8 - e^{12}m^4n^8 - e^{14}m^4n^8 - e^4m^6n^8 + e^6m^6n^8 + \\ &- e^8m^6n^8 + e^{10}m^6n^8 - e^{12}m^6n^8 + e^6m^8n^8 + e^8m^8n^8 + e^{10}m^8n^8 - e^{10}m^2n^{10} + \\ &+ e^4m^4n^{10} + e^6m^4n^{10} + 2e^8m^4n^{10} + 2e^{12}m^4n^{10} + e^{14}m^4n^{10} + e^{16}m^4n^{10} + \\ &+ 2e^6m^6n^{10} + 3e^{10}m^6n^{10} + 2e^{14}m^6n^{10} - 2e^8m^6n^{12} - 3e^{12}m^6n^{12} - 2e^{16}m^6n^{12} + \\ &- e^6m^8n^{12} - e^8m^8n^{12} - 2e^{10}m^8n^{12} - 2e^{14}m^8n^{12} - e^{16}m^8n^{12} - e^{18}m^8n^{12} + \\ &+ e^{12}m^{10}n^{12} - e^{12}m^4n^{14} - e^{14}m^4n^{14} - e^{16}m^4n^{14} + e^{10}m^6n^{14} - e^{12}m^6n^{14} + \\ &+ e^{14}m^6n^{14} - e^{16}m^6n^{14} + e^{18}m^6n^{14} + e^8m^8n^{14} + e^{10}m^8n^{14} + 3e^{12}m^8n^{14} + \\ &+ e^{14}m^8n^{14} + 3e^{16}m^8n^{14} + e^{18}m^8n^{14} + e^{20}m^8n^{14} + e^{10}m^{10}n^{14} + e^{12}m^{10}n^{14} + \\ &+ e^{14}m^{10}n^{14} + e^{16}m^{10}n^{14} + e^{18}m^{10}n^{14} + e^{12}m^6n^{16} + 2e^{14}m^6n^{16} + 2e^{16}m^6n^{16} + \\ &+ 2e^{18}m^6n^{16} + e^{20}m^6n^{16} + e^{12}m^8n^{16} + e^{14}m^8n^{16} + 3e^{16}m^8n^{16} + e^{18}m^8n^{16} + \\ &+ e^{20}m^8n^{16} - e^{12}m^{10}n^{16} - e^{20}m^{10}n^{16} - e^{14}m^8n^{18} - e^{16}m^8n^{18} - 2e^{18}m^8n^{18} + \\ &- e^{20}m^8n^{18} - e^{22}m^8n^{18} - 2e^{16}m^{10}n^{18} - 2e^{18}m^{10}n^{18} - 2e^{20}m^{10}n^{18} - e^{18}m^{12}n^{18} + \\ &+ e^{20}m^{12}n^{20} - e^{22}m^{12}n^{22}\,,\end{aligned} \tag{3.63}$$

$$\mathcal{D}(e,m,n) = \left(1-e^2\right)\left(1-m^2\right)\left(1-n^2\right)\left(1-e^4\right)\left(1-m^4\right)\left(1-n^4\right)\left(1-e^2n^2\right)^2 \times$$

$$\left(1-m^2n^2\right)\left(1-e^6\right)\left(1-e^2n^4\right)\left(1-e^4n^2\right)\left(1-m^2n^4\right)\times$$
$$\left(1-e^2m^2n^2\right)\left(1-e^4m^2n^2\right)\left(1-e^4m^2n^4\right)\left(1-e^8m^2n^4\right),$$

which in the single-graded limit have the following form

$$\begin{aligned}\mathcal{N}(q) &= 1+q^2+q^4+2q^6+6q^8+10q^{10}+18q^{12}+23q^{14}+28q^{16}+31q^{18}+34q^{20}+32q^{22}+\\ &+34q^{24}+31q^{26}+28q^{28}+23q^{30}+18q^{32}+10q^{34}+6q^{36}+2q^{38}+q^{40}+q^{42}+q^{44},\\ \mathcal{D}(q) &= \left(1-q^2\right)^2\left(1-q^4\right)^5\left(1-q^6\right)^4\left(1-q^8\right)\left(1-q^{10}\right)\left(1-q^{14}\right).\end{aligned} \tag{3.64}$$

The multi-graded plethystic logarithm is given by

$$\begin{aligned}\mathrm{PL}(e,m,n) &= e^2+m^2+n^2+e^4+m^4+e^2n^2+m^2n^2+n^4+e^6+e^4n^2+e^2m^2n^2+e^2n^4+\\ &+m^2n^4+e^4m^2n^2+e^4n^4+2e^2m^2n^4+m^4n^4+3e^4m^2n^4+e^2m^4n^4+e^2m^2n^6+\\ &+2e^6m^2n^4+2e^4m^4n^4+e^6n^6+2e^4m^2n^6+e^8m^2n^4+e^6m^4n^4+2e^6m^2n^6+\\ &-e^2m^6n^6-e^2m^4n^8+e^8m^4n^4+2e^8m^2n^6-e^6m^4n^6-2e^4m^6n^6-e^6m^2n^8+\\ &-5e^4m^4n^8-2e^2m^6n^8-m^8n^8+e^{10}m^2n^6-2e^6m^6n^6-e^8m^2n^8-8e^6m^4n^8+\\ &-6e^4m^6n^8-e^2m^8n^8-e^6m^2n^{10}-2e^4m^4n^{10}-e^2m^6n^{10}-\mathcal{O}([emn]^{20}).\end{aligned} \tag{3.65}$$

The plethystic logarithm is also non-terminating, indicating that the algebraic structure of the flavour invariants is that of a non-complete intersection ring. The pure negative order appears at $\mathcal{O}([emn]^{20})$, and the *generating* set can be obtained considering invariants up to $\mathcal{O}([emn]^{18})$ as shown in Ref. [252] or in terms of our invariants in Eq. (3.67).

3.C List of Invariants

Due to its length, we refer to Ref. [4] for the full set of invariants and will give the sets for a reduced number of flavours here. For the theory with $n_N = n_f = 2$, the *generating* set can be formed with the invariants

$$\text{Gen.}(n_N=n_f=2):\ \{\mathcal{I}_1,\mathcal{I}_2,\mathcal{I}_3,\mathcal{I}_4,\mathcal{I}_5,\mathcal{I}_6,\mathcal{I}_7,\mathcal{I}_8,\mathcal{I}_{14},\mathcal{I}_{17},\mathcal{I}_{22},\mathcal{I}_{35},\mathcal{J}_1,\mathcal{J}_2,\mathcal{J}_5,\mathcal{J}_7,\mathcal{J}_{28},\mathcal{J}_{31}\}, \tag{3.66}$$

which is also shown in Ref. [218] with a different convention. For the theory with $n_N = 2, n_f = 3$, the *generating* set is given by

$$\begin{aligned}\text{Gen.}(n_N=2,n_f=3):\ &\{\mathcal{I}_1,\mathcal{I}_2,\mathcal{I}_3,\mathcal{I}_4,\mathcal{I}_5,\mathcal{I}_6,\mathcal{I}_7,\mathcal{I}_8,\mathcal{I}_9,\mathcal{I}_{12},\mathcal{I}_{13},\mathcal{I}_{14},\mathcal{I}_{17},\mathcal{I}_{18},\mathcal{I}_{22},\mathcal{I}_{25},\\ &\mathcal{I}_{34},\mathcal{I}_{35},\mathcal{I}_{54},\mathcal{I}_{79},\mathcal{J}_1,\mathcal{J}_2,\mathcal{J}_5,\mathcal{J}_7,\mathcal{J}_9,\mathcal{J}_{10},\mathcal{J}_{26},\mathcal{J}_{28},\mathcal{J}_{29},\mathcal{J}_{31},\mathcal{J}_{32},\mathcal{J}_{68},\mathcal{J}_{70},\mathcal{J}_{72},\\ &\mathcal{J}_{132},\mathcal{J}_{133},\mathcal{J}_{134},\mathcal{J}_{195}\}.\end{aligned} \tag{3.67}$$

The above *generating* set has already been shown in Ref. [252], but the commutation notation is equivalently represented by taking imaginary part in our notation.

We can also easily identify that the primary invariants shown in Eq. (3.16) correspond to the invariants

$$\text{Primary set}: \{\mathcal{I}_1,\mathcal{I}_2,\mathcal{I}_3,\mathcal{I}_5,\mathcal{I}_6,\mathcal{I}_7,\mathcal{I}_8,\mathcal{I}_9,\mathcal{I}_{12},\mathcal{I}_{13},\mathcal{I}_{15},\mathcal{I}_{23},\mathcal{I}_{25},\mathcal{I}_{34},\mathcal{I}_{35},\mathcal{I}_{47},\mathcal{I}_{50},\mathcal{I}_{54},\mathcal{I}_{65},\mathcal{I}_{79},\mathcal{I}_{91}\}\,. \tag{3.68}$$

In the Dirac limit, the *generating* set will be reduced to have only 11 invariants, which are given by

$$\text{Gen.(Dirac limit)}: \{\mathcal{I}_1,\mathcal{I}_3,\mathcal{I}_4,\mathcal{I}_6,\mathcal{I}_7,\mathcal{I}_9,\mathcal{I}_{11},\mathcal{I}_{12},\mathcal{I}_{13},\mathcal{I}_{18},\mathcal{J}_{10}\}\,. \tag{3.69}$$

There is a one-to-one correspondence between these invariants and the invariants in the quark sector as shown in Eq. (2.98). For completeness, we also show the walk notations of generating flavour invariants in the quark sector, they are given by

$$\begin{aligned}\text{Gen.(Quark sector)}: \{&78, 89, 7878, 8989, 7898, 787878, 898989, 789898,\\ &787898, 78789898, \text{I@}787898789898\}\,.\end{aligned} \tag{3.70}$$

These walks are based on the graph shown in left bottom panel of Fig. 3.2.

3.D Hilbert's Nullstellensatz

Hilbert's Nullstellensatz [264–266], a fundamental result in algebraic geometry, establishes a profound connection between polynomial equations and the geometry of algebraic varieties. The traditional formulation of Hilbert's Nullstellensatz often involves a polynomial ring and its associated ideals. Consider the polynomial ring $R = k[x_1, x_2, \dots, x_n]$ in n variables over the field k (a mathematical structure that generalises the concept of numbers). This ring consists of polynomials in the variables $x_1, x_2, \dots, x_n$ with coefficients in k. We will now introduce the fundamental mathematical concepts required for presenting Hilbert's Nullstellensatz.

- Ideal

  An ideal I in the polynomial ring R is a subset of polynomials, which satisfies

$$\begin{aligned}&(1)\quad 0 \in I.\\ &(2)\quad \text{If } f, g \in I, \text{ then } f + g \in I.\\ &(3)\quad \text{If } f \in I \text{ and } g \in R, \text{ then } fg \in I.\end{aligned} \tag{3.71}$$

- Variety

  Given an ideal I, the variety $V(I)$ is the set of common zeros of all polynomials in I. Formally, a point $(a_1, a_2, \dots, a_n)$ lies in the variety $V(I)$ if and only if every polynomial in I evaluates to zero at that point

$$V(I) = \{(a_1, a_2, \dots, a_n) \mid f(a_1, a_2, \dots, a_n) = 0 \text{ for all } f \in I\}\,. \tag{3.72}$$

- Radical of an Ideal

The radical of an ideal I, denoted by $\sqrt{I}$, is the set of all polynomials g such that some power of g belongs to I. Mathematically, $\sqrt{I}$ is defined as

$$\sqrt{I} = \{g \mid g^k \in I \text{ for some } k \geq 1\} . \tag{3.73}$$

Hilbert's Nullstellensatz asserts that for any algebraically closed field k, there is a bijective correspondence between the points of a variety $V(I)$ and the radical ideals $\sqrt{I}$ defining the variety. Formally, this correspondence is expressed as

$$\text{Ideal}(V(I)) = \sqrt{I} , \tag{3.74}$$

where Ideal($V(I)$) denotes the ideal of polynomials vanishing on the variety $V(I)$.

In a more polynomial-centred language, Hilbert's Nullstellensatz can also be formulated differently. If a polynomial p vanishes on the variety $V(I)$, it belongs to Ideal($V(I)$), and, by Hilbert's Nullstellensatz as shown in Eq. (3.74), it also belongs to $\sqrt{I}$. According to the definition of $\sqrt{I}$, there exists $s \geq 1$ such that $p^s \in I$, which can thus be expressed as

$$p^s = f_1 p_1 + f_2 p_2 + \cdots + f_m p_m , \tag{3.75}$$

where $f_i \in \mathbb{R}$ and p_i are the defining polynomials of I. This equation essentially states that if p is vanishing under the common zeros of the defining polynomials of the ideal I, then some s-th power of the polynomial p can be expressed as a combination of these defining polynomials.

3.E CPC Conditions for $n_N = n_f = 2$

3.E.1 Minimal CPC Set for $n_N = n_f = 2$

The simplified model with two generations of fermions serves as a good example for the algebraic studies. In Ref. [218], the authors find the following 6 CP-odd invariants in the *generating* set

$$\begin{aligned}
J_1 &= \text{ImTr}\left(M_N Y_N^\dagger Y_N Y_N^\dagger Y_e Y_e^\dagger Y_N M_N^*\right) \sim \mathcal{J}_2 \\
J_2 &= \text{ImTr}\left(M_N^* M_N Y_N^\dagger Y_N M_N^* Y_N^T Y_N^* M_N\right) \sim \mathcal{J}_1 \\
J_3 &= \text{ImTr}\left(M_N^* M_N Y_N^\dagger Y_e Y_e^\dagger Y_N M_N^* Y_N^T Y_N^* M_N\right) \sim \mathcal{J}_7 \\
J_4 &= \text{ImTr}\left(M_N Y_N^\dagger Y_N Y_N^\dagger Y_e Y_e^\dagger Y_N M_N^* Y_N^T Y_N^*\right) \sim \mathcal{J}_5 \\
J_5 &= \text{ImTr}\left(M_N M_N^* M_N Y_N^\dagger Y_e Y_e^\dagger Y_N M_N^* Y_N^T Y_e^* Y_e^T Y_N^*\right) \sim \mathcal{J}_{31} \\
J_6 &= \text{ImTr}\left(M_N Y_N^\dagger Y_N Y_N^\dagger Y_e Y_e^\dagger Y_N M_N^* Y_N^T Y_e^* Y_e^T Y_N^*\right) \sim \mathcal{J}_{28}
\end{aligned} \tag{3.76}$$

which we have translated to our notation. Although the CP-odd generating set is small, it is still difficult to find the common zeros of the polynomials based on usual methods. However, the invariants can also be considered as ideals in the polynomial ring of the theory. In this section, we will analyse these ideals with the software package `Macaulay2` [263] based on the parameterisation in Eq. (3.48). To simplify the notation, we take $r_{11} = a, r_{21} = c, c_{12} = b + p\,i$ and $c_{22} = d + q\,i$. Therefore, the polynomial ring is defined as $R := \mathbb{Q}[y_e, y_\mu, m_1, m_2, a, b, c, d, p, q]$ and all CPV effects can be characterised by the ideal I defined by the six CP-odd invariants, i.e., $I \equiv \langle J_1, \ldots, J_6 \rangle$. The vanishing set denoted by $V(I)$ captures all the CPC conditions. The problem of finding common zeros is equivalent to finding the irreducible components of the ideal.

According to Hilbert's Nullstellensatz, the ideal of all polynomials that vanish on the common zero set $V(I)$ is the radical of the ideal $\sqrt{I}$, which can be calculated by the **radical** function in `Macaulay2`. The CPC conditions are captured by the minimal primes of the radical

$$\begin{aligned}&\{\langle q, p\rangle,\ \langle q, a\rangle,\ \langle p, c\rangle,\ \langle c, a\rangle,\ \langle c, b\rangle,\ \langle d, a\rangle,\ \langle d, b\rangle,\ \langle m_1, a\rangle,\ \langle m_1, c\rangle,\ \langle m_2, a\rangle,\ \langle m_2, c\rangle,\\ &\langle m_2, m_1\rangle,\ \langle m_1, y_e - y_\mu\rangle,\ \langle m_2, y_e - y_\mu\rangle,\ \langle m_1, d\,p - b\,q\rangle,\ \langle m_2, d\,p - b\,q\rangle,\\ &\langle m_1 - m_2, y_e - y_\mu\rangle,\ \langle y_e - y_\mu, a\,b + c\,d\rangle,\ \langle y_e - y_\mu, a\,p + c\,q\rangle,\\ &\langle m_1 - m_2, a\,b\,c^2 - a^2\,c\,d + b^2\,c\,d - a\,b\,d^2 + c\,d\,p^2 - a\,b\,q^2\rangle\}\,.\end{aligned} \tag{3.77}$$

These solutions have been simplified assuming physical values for all parameters. The CPC conditions can be obtained by setting the generators of the ideals to 0. For instance, the first ideal in the above set indicates that there is one condition $p = q = 0$ that can lead to CPC, which is just the trivial solution of vanishing phases. In the algebraic geometry picture, all these conditions are fundamental objects, and they correspond to points, lines, surfaces, etc. In addition, each of these conditions has a connection to the special spectrum and enlarged symmetries of the theory.

As we explore the CPC conditions using the `Macaulay2` package, we also find that without introducing J_3, we can still derive the CPC conditions in Eq. (3.77). This suggests that J_3 must be redundant when determining the CPC conditions. This is indeed observed by the syzygy approach based on Hilbert's Nullstellensatz. The redundant J_3 in our notation is $\mathcal{J}_7$ (refer to Eq. (3.76) for the mapping). If we use the *generating* set shown in Eq. (3.66), we can find the following syzygy

$$2\mathcal{J}_7^2 = (\mathcal{I}_2^2 - \mathcal{I}_5)\mathcal{J}_2^2 + 2\mathcal{J}_1\mathcal{J}_{31}\,. \tag{3.78}$$

Therefore, $\mathcal{J}_7$ vanishes given that $\mathcal{J}_1 = \mathcal{J}_2 = 0$. We have also attempted to find similar syzygies for other CP-odd invariants at their square order in the *generating* set. However, no other syzygy could be found, and we also observed that at higher orders, the syzygies are not easy to solve. Thus, we can conclude that the minimal CPC set is given by $\{J_1, J_2, J_4, J_5, J_6\}$ up to square order based on Hilbert's Nullstellensatz.

By analysing the polynomial ring, it is also possible to generate the conditions leading to a special spectrum with a larger exact symmetry group, yielding unphysical phases. The conditions leading to unphysical phase of p or q can be obtained by the elimination of variables, and the relevant function in `Macaulay2` is called **eliminate**. By eliminating the CP-odd variable p or q, one can find the following conditions

$$\begin{aligned}&\text{unphysical } p\text{: } \{\langle q\rangle,\ \langle c\rangle,\ \langle m_1\rangle,\ \langle m_2\rangle,\ \langle m_1-m_2\rangle,\ \langle y_e-y_\mu\rangle,\ \langle d,b\rangle,\ \langle d,a\rangle\}\,,\\ &\text{unphysical } q\text{: } \{\langle p\rangle,\ \langle a\rangle,\ \langle m_1\rangle,\ \langle m_2\rangle,\ \langle m_1-m_2\rangle,\ \langle y_e-y_\mu\rangle,\ \langle d,b\rangle,\ \langle c,b\rangle\}\,,\end{aligned} \tag{3.79}$$

where the unphysical conditions such as $\langle m_1+m_2\rangle$ is removed. The above conditions can also be calculated with the more physical parameterisation in Eq. (3.38). They are given as follows

$$\begin{aligned}\text{unphysical } \phi\text{: } &\{\langle\sin\varphi\rangle,\ \langle\sin\varphi-1\rangle,\ \langle\sin\varphi+1\rangle,\ \langle\sin\alpha\rangle,\ \langle\sin\alpha-1\rangle,\ \langle\sin\alpha+1\rangle,\\ &\langle m_1\rangle,\ \langle m_2\rangle,\ \langle m_1-m_2\rangle,\ \langle y_1-y_2\rangle\}\,,\\ \text{unphysical } \varphi\text{: } &\{\langle\sin\phi\rangle,\ \langle\sin\alpha\rangle,\ \langle\sin\alpha-1\rangle,\ \langle\sin\alpha+1\rangle,\ \langle\sin\theta\rangle,\ \langle\sin\theta-1\rangle,\\ &\langle\sin\theta+1\rangle,\ \langle y_e-y_\mu\rangle,\ \langle m_1-m_2\rangle,\ \langle y_1\rangle,\ \langle y_2\rangle,\ \langle y_1-y_2\rangle\}\,.\end{aligned} \tag{3.80}$$

By exploring these special conditions and their combinations, one can obtain all of the special spectra with enlarged symmetries that can be used to remove phases in the theory.

3.E.2 Pseudo-Real Couplings

There are some highly non-trivial conditions in the solution list in Eq. (3.77). For instance, the last one shows that the mass degeneracy of $m_1 = m_2$ and a vanishing of a specific combination of the matrix elements of Y_N can lead to CPC. One set of parameters that solves these conditions is

$$m_1 = m_2 = 1,\ y_e = 1,\ y_\mu = 2,\ a = 6,\ b = 2,\ c = 3,\ d = 4,\ p = 8,\ q = 5, \tag{3.81}$$

which corresponds to the following flavour matrices

$$Y_e = \begin{pmatrix}1 & 0\\ 0 & 2\end{pmatrix},\quad Y_N = \begin{pmatrix}6 & 2+8i\\ 3 & 4+5i\end{pmatrix},\quad M_N = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{3.82}$$

With this setup, we can check that all CP-odd invariants are vanishing, and there is no CP violation. However there are two complex numbers in Y_N, that cannot be made real by field redefinitions. Such a scenario of CP conservation in the presence of irremovable complex parameters was previously noted in Ref. [32, 33, 103] as pseudo-real couplings in the context of Three Higgs Doublet Models and toy models with complicated discrete symmetries. This can be understood as follows. Since M_N has degenerate eigenvalues, there is an $O(2)$ freedom for the field redefinition of N, while, because Y_e has non-degenerate eigenvalues, there is only a rephasing freedom for the field L. By applying these field redefinitions, we find that the phases in Y_N can not be removed. However, we can find the following field redefinition that can map Y_N to Y_N^*[15]

$$\begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{i\beta} \end{pmatrix} \begin{pmatrix} a & b+pi \\ c & d+qi \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} = \begin{pmatrix} a & b-pi \\ c & d-qi \end{pmatrix}. \tag{3.83}$$

Note that M_N and Y_e are real and diagonal in this basis, thus they are also mapped to their complex conjugate under this field redefinition. This indicates that the Lagrangian is symmetric under CP transformations up to a field redefinition, which is referred to as a generalised CP symmetry [268, 269]. Hence, even though there are irremovable phases present in the theory, CP is still conserved for this set of parameters. These special CPC conditions are correctly captured by the CP-odd flavour invariants, as they are all vanishing in these cases. In other words, all CPC conditions, no matter how special they may appear, can be obtained by setting CP-odd generating invariants to zero.

Note, that for a specific value of the rotation angle that solves Eq. (3.83) for the explicit example in Eq. (3.81), a discrete symmetry is defined that leaves the Lagrangian invariant. Furthermore, the generalised CP transformation that imposes Eq. (3.83), is of order 2, since both the rephasing matrix and the rotation matrix fulfil $AA^* = \mathbb{1}$, indicating a trivial flavour symmetry. There are additional cases in Eq. (3.77) that result in pseudo-real couplings. For example, one can verify that the ideal $\langle y_e - y_\mu, a\,p + c\,q\rangle$ corresponds to another discrete symmetry that leads to pseudo-real couplings. In general, if the condition involves the phases non-trivially, meaning the phases can be set to certain constrained non-zero values, the couplings will be pseudo-real in such scenarios.

[15]For the choice of parameters shown in Eq. (3.81), we find $\theta = 2\arctan(3)$, $\alpha = \pi + \arctan(4/3)$, $\beta = 3\pi/2$.

4 The Flavour Invariants of the SMEFT with Massive Neutrinos

In Sec. 2.2.3, we have introduced CP-odd flavour invariants capturing all sources of CP violation in the SMEFT at dimension 6, following the discussion in Refs. [103, 104]. There, we have neglected all neutrino masses, which is incompatible with our observation of massive neutrinos in Nature. We have already introduced the most popular possibilities for generating neutrino masses in Sec. 2.3 and constructed their generating set of flavour invariants in Chap. 3. In this section, we want to extend this discussion to the non-renormalisable interactions.

There are three different possibilities we want to discuss. First, we want to consider the option of leaving right-handed sterile neutrinos aside and generating a Majorana mass term for the left-handed SM neutrinos through the Weinberg operator, which is generated by some heavy lepton number-violating new physics. Subsequently, we will consider the EFT of the νSM, which we have studied in Chap. 3. Here, we will differentiate two cases: in the first case, we will not allow for lepton number-breaking terms in the Lagrangian; hence, only Dirac neutrino masses are allowed. In the second case, we will also allow for Majorana masses for the sterile right-handed neutrino.

4.1 The Weinberg Operator

Let us start with the pure SMEFT case, where now the Weinberg operator

$$\mathcal{O}_5 = \left(\bar{L}^c \tilde{H}^*\right)\left(\tilde{H}^\dagger L\right), \tag{4.1}$$

at dimension 5 is allowed, which we have ignored previously due to its breaking of lepton number. For an anti-symmetric charge conjugation matrix C, the Wilson coefficient C_5 of the Weinberg operator is a symmetric matrix and hence, contains 6 CP-even and 6 CP-odd parameters. Due to its transformation properties under the $U(3)_L$ flavour group[1]

$$C_5 \sim (\bar{\mathbf{3}}_{\mathbf{L}} \otimes_s \bar{\mathbf{3}}_{\mathbf{L}})_{-2} \,, \tag{4.2}$$

where the representations are those of the non-Abelian part of the flavour group, $\otimes_s$ is the symmetric tensor product of the simple representations and the subscript denotes the Abelian flavour charge, the flavour invariants of the Weinberg operator in the presence of all other SM and SMEFT dimension-6 operators have to be at least quadratic in C_5. Indeed, we can write down the following generic form for the invariants

$$I^{(2)}_{ab} = \mathrm{Tr}\left(C_5 X_e^a C_5^* X_e^{*b}\right) \,, \tag{4.3}$$

where $X_e = Y_e Y_e^\dagger$ and $a, b = 0, 1, 2$, since any higher power can be removed by virtue of the Cayley–Hamilton theorem. It turns out that all of these invariants are real, i.e. at dimension 6 there exist no flavour-invariant sources of CP violation in the Weinberg operator. This is easy to show by computing the conjugate of the invariant

$$\left(I^{(2)}_{ab}\right)^* = \mathrm{Tr}\left(\left(C_5 X_e^a C_5^* X_e^{*b}\right)^\dagger\right) = \mathrm{Tr}\left(X_e^{*b} C_5 X_e^a C_5^*\right) = \mathrm{Tr}\left(C_5 X_e^a C_5^* X_e^{*b}\right) = I^{(2)}_{a,b} \tag{4.4}$$

where we have used $\mathrm{Tr}(A) = \mathrm{Tr}\big(A^T\big)$, the fact that C_5 and X_e are symmetric and hermitian, respectively, and the cyclic property of the trace.

Due to the transformations properties of C_5, more invariants can only be written down by using four insertions of C_5 and its conjugate. These invariants can be written in the following generic form

$$I^{(4)}_{abcd} = \mathrm{Tr}\left(C_5 X_e^a C_5^* X_e^{*b} C_5 X_e^c C_5^* X_e^{*d}\right) \,, \tag{4.5}$$

where again $a, b, c, d = 0, 1, 2$. Only now, some of the invariants have imaginary parts and hence, capture sources of CP violation. Since the invariants are no longer linear in the Wilson coefficients, we can no longer directly make use of linear algebra to check the independence of the invariants. We can however still define a transfer matrix by spanning a vector space with all possible imaginary combinations of 4 entries of the C_5, which are exactly the terms appearing in $I^{(4)}_{a,b,c,d}$. For instance, taking the Wilson coefficient vector in Eq. (2.36) to have the entries of the form $\mathrm{Im}\,(C)^3\,\mathrm{Re}\,(C)$ and $\mathrm{Im}\,(C)\,\mathrm{Re}\,(C)^3$, while all other terms correspond to the real block of the transfer matrix. Computing the rank of the transfer matrix for the invariants of the structure in Eq. (4.5), one find that the set

$$I^{(4)}_{1100}\,, \quad I^{(4)}_{1200}\,, \quad I^{(4)}_{2200}\,, \quad I^{(4)}_{0112}\,, \quad I^{(4)}_{0122}\,, \quad I^{(4)}_{1122}\,, \tag{4.6}$$

captures the necessary and sufficient condition for CP conservation in the SM extended with the Weinberg operator. Note, that if one goes to this order in the EFT expansion also flavour invariants with single insertions of the Wilson coefficient of dimension-8 operators, double insertions of the Wilson coefficient of dimension-6 operators and double insertions of

[1]The operator is a singlet under the remaining subgroups of the $U(3)^5$ flavour group of the SM.

the Wilson coefficient of the Weinberg operator with the insertion of the Wilson coefficient of dimension-6 operators should be considered. For instance, considering the Yukawa-like operator C_{eH}, we can write

$$\mathrm{Tr}\left(C_5 X_e^a C_{eH} Y_e^\dagger X_e^b C_5^* X_e^{*c}\right) , \tag{4.7}$$

capturing the sources of CP violation in the interference between an operator insertion of $\mathcal{O}_{Hl}^{(1)}$ and twice the Weinberg operator in a given observable. Here, one should keep in mind that all necessary and sufficient condition for CP conservation are already captured by the previously considered invariants. However, the additional invariants could still appear in computations and capture sources of CP violation in a certain way that is not captured by the previously considered invariants.

4.2 Sterile Neutrinos with Lepton Number Conservation

As alluded to at the beginning of this chapter, another possibility to generate neutrino masses is to add right-handed sterile neutrinos to the theory. Assuming that all particle masses are light, the right-handed neutrinos should be added to the low-energy particle spectrum, which has to be taken into account when constructing the EFT of the theory. Since the right-handed neutrinos are singlets under the SM gauge group, a Majorana mass term is in principle allowed for the Weyl fermion, breaking the accidental lepton number rephasing symmetry of the renormalisable SM. Therefore, we will split the analysis into two parts. First, we consider lepton number to be a good symmetry of the SM Lagrangian extended with the right-handed neutrino N as well. The remaining Lagrangian is that of the νSM introduced in Eq. (2.43) with M_N set to zero

$$\mathcal{L}_{\nu\mathrm{SM,Dirac}} = \mathcal{L}_{\mathrm{SM}} + \bar{N} i \partial\!\!\!/ N - \left(\bar{L} Y_N \tilde{H} N + \mathrm{h.c.}\right) , \tag{4.8}$$

which after EWSB gives rise to a Dirac neutrino mass. Note also, that adding a lepton number-conserving right-handed neutrino to the SM Lagrangian essentially makes the lepton Yukawa sector a copy of the quark Yukawa sector. The relevant operators of the νSMEFT in the case of conserved lepton number are those in Tab. 4.2 without those labelled by $\not{L}$.

In this case, we can simply recycle some of the results from Ref. [103], where the CP-odd flavour invariants with the non-trivial flavour structure of the quark sector was discussed. One thing should be kept in mind here. In Ref. [103], a Froggatt-Nielsen (FN) model [270] was utilised to organise the flavour sector of the SM and SMEFT flavourful interactions. We will introduce the model in more detail later, but the main points can be summarised as follows. In the FN construction a complex singlet scalar is postulated in the UV, which has a fixed charge of −1 under a new global $U(1)$ group. The components of the SM fermion flavour multiplets take different charges under the $U(1)$ group such that effective operators of the fermions with the new scalar are generated by demanding that the Lagrangian be invariant under the action of the new $U(1)$. The $U(1)$ is then spontaneously broken by the VEV of the scalar field, such that the VEV divided by the scale, where the effective operators between the scalar and the SM fermions are UV completed, matches $\lambda = \sin\theta_c \sim 0.22$ (with θ_c the Cabibbo angle) reproducing the SM flavour structure. In Ref. [103], this construction is extended to the non-renormalisable interactions of the SMEFT, such that the hierarchies in the flavour sector are explained by a single parameter. This parameter can be used to organise the flavour invariants by their leading power in λ.

In the lepton sector of the νSMEFT this is no longer possible, since the values of the neutrino masses (and their Majorana or Dirac character) are unknown. Hence, any FN model would be extremely model-dependent. Hence, we have to find another way to organise the importance of the flavour invariants of the νSMEFT. We will do this in a second below. Let us first discuss what we can learn about the CP-odd νSMEFT invariants at dimension 6 from the results of Ref. [103].

Let us start by counting the CP-odd parameters of the lepton number-conserving dimension-6 operators in the νSMEFT in Tab. 4.2. The operators $\mathcal{O}_{LNH}, \mathcal{O}_{HNe}, \mathcal{O}_{NW}$ and $\mathcal{O}_{NB}$ are all generic operators with one fermion bilinear. Hence, they each have 9 CP-odd parameters. In addition, the hermitian operator $\mathcal{O}_{HN}$ has 3 CP-odd parameters. The 4-fermion operators can be categorised as follows. The operators $\mathcal{O}_{duNe}, \mathcal{O}_{LNLe}, \mathcal{O}_{LNQd}, \mathcal{O}_{LdQN}$ and $\mathcal{O}_{QuNL}$ are generic 4-fermion operators without any symmetry relations; hence they each come with 81 CP-odd parameters. The operators $\mathcal{O}_{eN}, \mathcal{O}_{uN}, \mathcal{O}_{dN}, \mathcal{O}_{LN}$ and $\mathcal{O}_{QN}$ are “hermitian”, i.e. $C_{ijkl} = C^*_{jilk}$. They each come with 36 CP-odd parameters. Due to only N appearing in $\mathcal{O}_{NN}$ this “hermitian” operator has the following other symmetries $C_{ijkl} = C_{kjil} = C_{ilkj} = C_{klij}$ due to Fierz identity and the fact that the two currents can trivially be exchanged; hence the Wilson coefficient of the operator only contains 15 CP-odd parameters. In total, we have 639 CP-odd parameters in the Wilson coefficients of the dimension-6 lepton number-conserving νSMEFT[2]. Applying the findings of Ref. [103], we can make the qualitative statement that all of these phases are primary phases, which can be written down in a flavour basis-invariant way as the imaginary part of a trace of combinations of νSM Yukawa couplings and a single insertion of the Wilson coefficient. Those are the physical phases, that can appear in the interference term between the renormalisable and non-renormalisable contribution to an amplitude, schematically shown in Eq. (2.35). Together with the results derived in Chap. 3, this construction allows us to impose the conditions for CP conservation at the renormalisable level of the theory. Then, all the remaining conditions formulated as imaginary flavour invariants captures the true sources of CP violation in the UV parameterised in the νSMEFT.

In order to explicitly construct the invariants, an organising principle similar to the FN model for the SMEFT has to be chosen, such that for a given operator a set of invariants out of all possible constructible invariants can be selected parameterising the leading flavour-invariant phases of the effective operator. The FN model was a good choice for the SMEFT, as it parameterised the flavour hierarchy of the SM in the single parameter λ singling out the invariants that yield a complete set with maximal rank at the lowest possible order in λ. We briefly want to discuss several choices for an organising principle of the νSMEFT invariants here.

[2] This number corresponds to the operators, where at least one right-handed neutrino fields appears in the effective operators. The SMEFT operators, which technically are also part of the νSMEFT are not included in this number.

Even though the flavour charges of an FN model cannot be fixed like in the SM fermion sector due to the lack of knowledge about the mass generation of neutrino masses, one can make well-motivated assumptions about the neutrino mass spectrum and its origin to construct a generalised FN model that also includes the neutrino sector along the lines of what was, for instance, done in Ref. [271]. This would be the natural generalisation of the analysis performed in Refs. [103, 104] even though a large model dependence is introduced thanks to our ignorance of the neutrino mass spectrum.

Another possibility is to simply count the insertions of couplings in the flavour invariants. This is motivated by the less hierarchical PMNS mixing matrix in the neutrino sector, which unlike in the SM quark sector would lead to less drastic suppression of higher order invariants in the Yukawa couplings, determined by powers of λ in the FN-type models. Furthermore, if these invariants are expected to be generated in perturbation theory, more insertions of Yukawa couplings would naturally correspond to a higher loop suppression. Here, one obstacle would arise when the lepton number-breaking Majorana mass is taken into account: should an insertion of the Majorana mass M_N (divided by the only other scale in the problem v to make it dimensionless) be prioritised over an insertion of Y_N or vice-versa?

We will finish the discussion by constructing a complete set of flavour invariants for the class of operators, which have a single chirality-changing bilinear, i.e. the operators $\mathcal{O}_{LNH}, \mathcal{O}_{HNe}, \mathcal{O}_{NW}$ and $\mathcal{O}_{NB}$, taking $\mathcal{O}_{NB}$ as a proxy. Following Ref. [103], we define the generic invariant

$$L_{abcd}(C) = \operatorname{Im}\operatorname{Tr}\left(X_N^a X_e^b X_N^c X_e^d C\right) , \tag{4.9}$$

where $a, b, c, d = 0, 1, 2$. Then a complete set of invariants for the class of chirality-flipping single-bilinear operators is

$$\begin{aligned}
&L_{0000}(C_{NB}Y_N^\dagger), \quad L_{1000}(C_{NB}Y_N^\dagger), \quad L_{0100}(C_{NB}Y_N^\dagger), \\
&L_{1100}(C_{NB}Y_N^\dagger), \quad L_{0110}(C_{NB}Y_N^\dagger), \quad L_{2200}(C_{NB}Y_N^\dagger), \\
&L_{0220}(C_{NB}Y_N^\dagger), \quad L_{1220}(C_{NB}Y_N^\dagger), \quad L_{0112}(C_{NB}Y_N^\dagger).
\end{aligned}$$

Here, we have made the assumption that, in the spirit of the Jarlskog invariant, the invariants should also capture cases of degenerate Yukawa eigenvalues as well as texture zeros in the CKM matrix. Then for instance, the inclusion of both $L_{1000}(C_{NB}Y_N^\dagger)$ and $L_{2000}(C_{NB}Y_N^\dagger)$ is not allowed because they are related by a syzygy in the limit where $y_t \to 0$, even though no enlarged exact flavour symmetry of the renormalisable SM Lagrangian exists in this limit, that would allow for the removal of one of the complex parameters in C_{NB}. All phases in all other Wilson coefficients are also physical and a complete set of single-trace flavour invariants can be constructed for them. The explicit construction of a complete set based on one of the criteria laid out above is left for future work.

4.3 Sterile Neutrinos without Lepton Number Conservation

In this section, we will allow for lepton number-breaking terms in the Lagrangian. Then, the renormalisable Lagrangian will be that of the full νSM including the Majorana mass term

$$\mathcal{L}_{\nu\text{SM}} = \mathcal{L}_{\text{SM}} + \bar{N}i\partial\!\!\!/ N - \left(\frac{1}{2}\bar{N}^c M_N N + \bar{L}Y_N\tilde{H}N + \text{h.c.}\right) . \tag{4.10}$$

In addition, more operators are allowed at the non-renormalisable level already at mass dimension 5. These operators can be found in Tab. 4.1. For an anti-hermitian charge parity matrix C the Wilson coefficient of the operator $\mathcal{O}_N$ is symmetric, i.e. it has 6 CP-odd parameters, and the Wilson coefficient of the operator $\mathcal{O}_{NNB}$ is anti-symmetric, i.e. it has 3 CP-odd parameters. In Sec. 4.1, the Weinberg operator which has a similar fermion structure could not built flavour invariants at the linear order in the Wilson coefficient due to the absence of a lepton number-breaking interaction in the renormalisable SM Lagrangian. This changes in the νSM with lepton number breaking. The 9 CP-odd parameters of the two operators can all be captured in terms of flavour invariants as we will show in a second. Another comment is in order about the Weinberg operator $\mathcal{O}_5$. Using the renormalisable couplings of the νSM, we can construct the following object

$$Y_N^T C_5 Y_N \sim M_N \sim (\bar{3}_N \otimes_s \bar{3}_N)_{-2} , \tag{4.11}$$

that transforms in the same way as the Majorana matrix under the flavour group. Hence, using M_N, one can build CP-odd invariants at the leading order in C_5. Defining $\tilde{X}_N = Y_N^\dagger Y_N$, which transforms as a $\bar{3} \otimes 3$ under $U(3)_N$, as well as $X_M = M_N M_N^\dagger$, we can write down the following invariants

$$L_{abcd}(Y_N^T C_5 Y_N) = \text{Im}\,\text{Tr}\left(\tilde{X}_N^a X_M^b \tilde{X}_N^c X_M^d\, Y_N^T C_5 Y_N\right) \tag{4.12}$$

In the presence of a Majorana mass term and lepton number-violating operators of the νSMEFT for some operators no closed form for the invariants exists. Then, it can be useful to use the graph-based methods introduced in Chap. 3 to construct the invariants systematically. The corresponding graph for C_5 can be found in Fig. 4.1. Using the transfer matrix method for the invariants in $L_{abcd}(Y_N^T C_5 Y_N)$ allows for the construction of a complete set of primary invariants for C_5 in the presence of sterile neutrinos with a Majorana mass term.

Assuming that baryon number is still a good symmetry, one more operator can be constructed at dimension 6, which we have labelled as $\mathcal{O}_{NNNN}$ in Tab. 4.2. This operator has many redundancies ($\mathcal{O}_{ijkl} = \mathcal{O}_{klij} = \mathcal{O}_{jikl} = -\mathcal{O}_{iklj} - \mathcal{O}_{iljk}$) due to the exchange of the two currents, the hermiticity of the Wilson coefficients and a Fierz identity. Hence, this 4-fermion operator only contains 6 CP-odd phases, which can all be captured by flavour-invariants at the leading order in the Wilson coefficient.

Hence, comparing with Sec. 4.2, 15 more phases appear by allowing for lepton number violation, which together with the renormalisable parameters of the νSM can all be expressed as flavour invariants linear in the Wilson coefficients. In addition, the lepton number-breaking

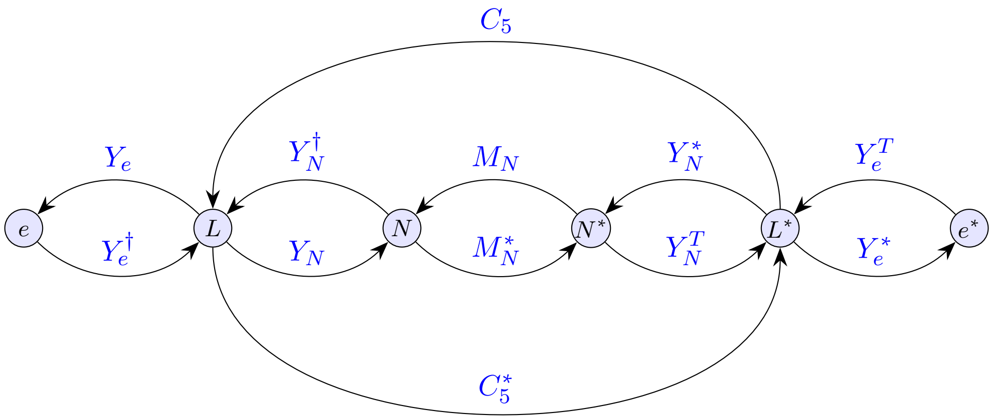


Figure 4.1: The flavour invariant graph for the Wilson coefficient of the SMEFT Weinberg operator $\mathcal{O}_5$ in the presence of sterile neutrinos with a Majorana mass term.

Majorana mass term of the sterile neutrino permits the construction of CP-odd invariants of the Weinberg operator for all 6 phases contained in the Weinberg operator.

Appendices to Chapter 4

4.A List of νSMEFT Operators

$\psi^2 H^2$		$\psi^2 X$	
$\mathcal{O}_N$	$H^\dagger H \bar{N}^c N$	$\mathcal{O}_{NNB}$	$\bar{N}^c \sigma^{\mu\nu} N B_{\mu\nu}$

Table 4.1: Dimension-5 operators of the νSMEFT, the SMEFT extended with three generations of light right-handed sterile neutrinos [272]. Both of these operators break lepton number. Only operators with at least one right-handed neutrino field are kept.

$\psi^2 H^3$ + h.c.		ψ^4	
$\mathcal{O}_{LNH}$	$(\bar{L}\tilde{H}N)(H^\dagger H)$	$\mathcal{O}_{NN}$	$(\bar{N}\gamma^\mu N)(\bar{N}\gamma_\mu N)$
$\psi^2 H^2 D$		$\mathcal{O}_{eN}$	$(\bar{e}\gamma^\mu e)(\bar{N}\gamma_\mu N)$
$\mathcal{O}_{HN}$	$(\bar{N}\gamma^\mu N)(H^\dagger i\overleftrightarrow{D}_\mu H)$	$\mathcal{O}_{uN}$	$(\bar{u}\gamma^\mu u)(\bar{N}\gamma_\mu N)$
$\mathcal{O}_{HNe}$(+h.c.)	$(\bar{N}\gamma^\mu e)(\tilde{H}^\dagger i D_\mu H)$	$\mathcal{O}_{dN}$	$(\bar{d}\gamma^\mu d)(\bar{N}\gamma_\mu N)$
$\psi^2 H X$ + h.c.		$\mathcal{O}_{duNe}$(+h.c.)	$(\bar{d}\gamma^\mu u)(\bar{N}\gamma_\mu e)$
$\mathcal{O}_{NW}$	$(\bar{L}\sigma_{\mu\nu}N)\tau^I \tilde{H} W^{I\mu\nu}$	$\mathcal{O}_{LN}$	$(\bar{L}\gamma^\mu L)(\bar{N}\gamma_\mu N)$
$\mathcal{O}_{NB}$	$(\bar{L}\sigma_{\mu\nu}N)\tilde{H} B^{\mu\nu}$	$\mathcal{O}_{QN}$	$(\bar{Q}\gamma^\mu Q)(\bar{N}\gamma_\mu N)$
$\not{L} \cap B$ + h.c.		$\mathcal{O}_{LNLe}$(+h.c.)	$(\bar{L}N)\epsilon(\bar{L}e)$
$\mathcal{O}_{NNNN}$	$(\bar{N}^c N)(\bar{N}^c N)$	$\mathcal{O}_{LNQd}$(+h.c.)	$(\bar{L}N)\epsilon(\bar{Q}d))$
$\not{L} \cap \not{B}$ + h.c.		$\mathcal{O}_{LdQN}$(+h.c.)	$(\bar{L}d)\epsilon(\bar{Q}N)$
$\mathcal{O}_{QQdN}$	$\epsilon_{ij}\epsilon_{\alpha\beta\sigma}(Q^i_\alpha C Q^j_\beta)(\bar{d}^c_\sigma N)$	$\mathcal{O}_{QuNL}$(+h.c.)	$(\bar{Q}u)(\bar{N}L)$
$\mathcal{O}_{uddN}$	$\epsilon_{\alpha\beta\sigma}(\bar{u}^c_\alpha d_\beta)(\bar{d}^c_\sigma N)$		

Table 4.2: Dimension-6 operators of the νSMEFT, the SMEFT extended with three generations of light right-handed sterile neutrinos. Only operators with at least one right-handed neutrino field are kept. Adapted from Ref. [272].

5

Conclusions to Part I

In the first half of Part I of this thesis, we have studied the algebraic structure of the flavourful couplings of the νSM, the SM extended with three generations of sterile neutrinos, by constructing its set of generating flavour invariants. As a guide for the construction of the invariants, we have first calculated the Hilbert series and plethystic logarithm of the flavour invariants. Unlike the quark sector of the theory, whose flavourful couplings form a complete intersection ring, the lepton sector of the νSM forms a non-complete intersection ring and care has to be taken in the interpretation of the coefficients in the plethystic logarithm. In a non-complete intersection ring, the otherwise well-separated regions with positive terms – indicating the number of generating invariants of the theory at each order in the spurions – can overlap with the negative terms – indicating the number of syzygies among the generating invariants at each order in the spurions, leading to cancellations.

Therefore, we have approached the construction of the invariants using a brute force algorithm centred around a graph-based method, which maps all single-trace invariants to a unique graph and vice-versa. Then, all invariants in the theory can be constructed based on the graphs and reduced to a generating set by finding the explicit relations among the invariants with a numerical algorithm. By also keeping track of the syzygies among the generating invariants, which can be found with the same algorithm, the number of generating invariants and syzygies can be cross-checked against the plethystic logarithm order by order in the spurions. We find that the generating set consists of 459 invariants, out of which 208 are CP-even and 251 are CP-odd. The generating set can be further reduced to a primary set of 21 invariants, which captures the physical parameters in the νSM Lagrangian.

Since the seesaw models of type-I and type-III have the same flavour structure as the νSM, we can use the flavour invariants to study the seesaw limit. This is done by identifying M_N^{-1} appearing in the seesaw limit with M_N^*, present in our generating set of invariants. Considering structures in the flavour invariants that match to the Wilson coefficients at the leading and next-to leading order in the seesaw EFT, we showed that 12 and 21 parameters, respectively, are captured by the reduced generating set. Here, the number 12 corresponds to the number of masses, mixing angles and phases in the low-energy theory leptons, while the remaining parameters are captured by effective operators in the low-energy theory. If the power counting of the EFT, i.e. the total suppression of the invariants with the Majorana mass, is also taken into account, we find that the 12 and 21 physical parameters can only be captured in a flavour-invariant way with a total suppression of two and four powers of the Majorana mass.

In the spirit of the Jarlskog invariant, we have defined a minimal set of CP-odd flavour invariants, the minimal CPC set, that captures the necessary and sufficient conditions for conservation of CP in a flavour-invariant way, independent of a flavour basis or any assumptions about the parameter spectrum of the theory. This is particularly interesting for the neutrino sector because the parameters of the theory of neutrino mass generation are only known to low precision or for some only upper bounds exist. Reducing the set of CP-odd generating invariants to a minimal set is a difficult task, which we only managed to complete for the theory with two generations of leptons, while the three generation case was impossible to complete by our means. The roots of the flavour invariants in the minimal CPC set of the two generations case allowed us to identify an interesting set of pseudoreal couplings featuring phases, which are not removable by flavour transformations, while the theory is still CP-conserving. This can be appreciated in a straightforward way using the CP-odd flavour invariants, which all vanish when evaluated on this set of couplings.

In the second half of the first part of this thesis, we have extended the results of Chap. 3 to the couplings in the effective interactions of the theory. In a first step, we considered the SMEFT in the presence of neutrino masses through the Weinberg operator. There, we have found that the parameters in the Wilson coefficient of the dimension-5 Weinberg operator can only appear in a flavour-invariant way at dimension 6 and in particular, the phases in the Weinberg operator can only appear at dimension 8 as flavour invariants.

Then, we have added right-handed sterile neutrinos to the field content corresponding to the νSMEFT, both with and without lepton number breaking. In the Dirac case, where only lepton number-conserving interactions are added, the νSMEFT has the same structure as the quark sector of the SMEFT. Therefore, the classification of the invariants follows the same reasoning as the one of the SMEFT CP-odd invariants. The only point that has to be addressed is that the ordering principle used for the SMEFT – a Froggatt-Nielsen model – has to be changed, as there does not exist a working Frogatt–Nielsen model in the neutrino sector due to the lack of knowledge about the parameters to be described. We have suggested alternatives that will be used in a more complete analysis of the νSMEFT invariants. Note, that in the SMEFT some phases in the Wilson coefficients of the leptonic operators could not appear in a flavour-invariant way at the leading order in the EFT with only one insertion of the Wilson coefficient. This changes in the presence of the Yukawa coupling of the SM fields to the right-handed neutrinos in the flavour invariants, which breaks lepton *family* number allowing to project out more phases from the leptonic SMEFT Wilson coefficients. Then, all phases of the leptonic SMEFT operators can be expressed in a flavour-invariant way with only one insertion of the Wilson coefficient. In addition, the νSMEFT has more operators with right-handed sterile neutrino. We have argued, that all phases of these Wilson coefficients can appear in a flavour-invariant way with only one insertion of the Wilson coefficient.

When a Majorana mass term is added, the same is also true for the νSMEFT operators breaking lepton number: all phases appearing in the Wilson coefficients of these operators can be written in a flavour-invariant way with only one insertion of the Wilson coefficient.

Furthermore, due to the additional source of lepton number-breaking through the Majorana mass, the phases in the SMEFT Weinberg operator can now also appear in a flavour-invariant way with only one insertion of the Wilson coefficient of the Weinberg operator.

The work presented in the first part of this thesis can be extended in several ways. First, it would be interesting to connect the invariants of both the νSM and νSMEFT to observables. One good candidate is the difference between the oscillation probabilities of neutrinos and their antineutrinos, which as shown in Eq. (2.50) should be proportional to the CP-odd invariants of the theory. Furthermore, as already announced in Sec. 4.2, a complete analysis of the CP-odd flavour invariants will appear in a future publication.

Part II

Symmetry Breaking in ALP EFTs

6 The Shift-Invariant Orders of an Axionlike Particle

6.1 Introduction

As alluded to in Sec. 2.4, axions are a prime candidate to settling the strong CP problem, while at the same time also solving the dark matter problem and are prevalent in many BSM models. A vital property of ALPs in solving these issues is their pNGB nature, realised by an approximate shift symmetry of the axion field. This shift symmetry allows axions to receive their potential from QCD, enabling the resolution of the strong CP problem and making the axion a good candidate for (ultra-)light dark matter [144]. The presence of these features depends on the parametrically closeness to a shift-symmetric point and the desired features become more exact as the point is approached.

On the other hand, there are also good reasons to study some explicit breaking of the symmetry. For instance, quantum gravity does not allow for exact global symmetries (see Sec. 2.4) leading to Planck scale-suppressed corrections[1] to the axion potential and its interactions with other particles. Suppressing these interactions is necessary in any model with pNGBs and goes under the name of axion quality problem. Furthermore, shift breaking can be a key aspect of model building: In the relaxion mechanism [274, 275] an explicit breaking term is needed to scan the Higgs mass parameter and resolve the Higgs hierarchy problem. Shift-breaking scalars have also been used in the study of collider anomalies [276]. Therefore, it is important to study these effects both from a phenomenological and more formal point of view. As axions can appear in a multitude of well-motivated BSM theories, it is convenient to work with the EFT introduced in Sec. 2.4.3.

As pNGBs, axions are generically light and can therefore be produced and contribute to processes at all energy scales of interest for high-energy physics. In addition, they arise in very diverse UV models, and can couple to all particles of the SM in all the ways compatible with their pNGB nature. Therefore, in a bottom-up approach, their couplings are essentially free parameters, up to the constraints imposed by the pNGB shift symmetry, which is precisely what an EFT approach encodes. For these reasons, axion EFTs have been systematically

[1] These effects can become much larger than naively expected when heavy particles are present in the UV above the scale of spontaneous PQ-breaking. Integrating them out can significantly lower the scale of gravity-induced breaking effects [273] worsening the axion quality problem.

studied since the early days of axion physics [172, 175], and are for instance used in the context of flavour physics [177–191] or LHC observables [192–211].

In this chapter, we want to systematically study the effects of the breaking of the axion shift invariance due to the axion couplings to SM fermions. We will work in the Yukawa basis introduced in Sec. 2.4.3, for which we will repeat the relevant part here for convenience

$$\mathcal{L} = \mathcal{L}_{\rm SM} + \frac{1}{2}\left(\partial_\mu a\right)\left(\partial^\mu a\right) - \frac{m_{a,0}^2}{2}a^2 - \frac{a}{f}\left(\bar{Q}\tilde{Y}_u\tilde{H}u + \bar{Q}\tilde{Y}_d H d + \bar{L}\tilde{Y}_e H e + \text{h.c.}\right) + \mathcal{O}\left(\frac{1}{f^2}\right) \,, \quad (6.1)$$

where f is the axion decay constant (we henceforth take $f \gg v$, the electroweak scale), $\tilde{Y}_{u,d,e}$ are *generic complex* matrices in flavour space, $\tilde{H} \equiv i\sigma^2 H^*$ and $\mathcal{L}_{\rm SM}$ contains the SM couplings, whose fermionic sector reads

$$\mathcal{L}_{\rm SM} \supset \sum_{\psi\in\rm SM} i\bar{\psi}\not{D}\psi - \left(\bar{Q}Y_u\tilde{H}u + \bar{Q}Y_d H d + \bar{L}Y_e H e + \text{h.c.}\right) \,. \quad (6.2)$$

The axion couplings in Eq. (6.1) do not preserve shift symmetry in general. The main goal of this chapter is to construct simple relations which allow us to identify when these couplings can be interpreted as the shift-invariant couplings of an axion, and also quantify the deviations from the shift-symmetric point.

As shown in Sec. 2.4.3, this question is usually answered by starting from the Lagrangian where the axion is derivatively coupled to fermions, making the axion shift symmetry $a \to a + \epsilon f$ manifest

$$\mathcal{L} = \mathcal{L}_{\rm SM} + \frac{1}{2}\left(\partial_\mu a\right)\left(\partial^\mu a\right) + \frac{\partial_\mu a}{f}\sum_{\psi\in\rm SM}\bar{\psi}c_\psi\gamma^\mu\psi + \mathcal{O}\left(\frac{1}{f^2}\right) \,, \quad (6.3)$$

and performing a field redefinition that maps the Wilson coefficients of the Lagrangian in Eq. (6.3) to those of Eq. (6.1) imposing the constraints on the couplings [212, 213]. These constraints can also be understood only in terms of the operator basis of Eq. (6.1), where the shift invariance is never manifest, by absorbing a shift of the axion via appropriate field redefinitions of the fermions [213].

As we will see in a second there are severe issues with these conditions: given a set of couplings, one has to check whether a set of complicated matrix equations can be solved. In addition, they do not allow to differentiate between approximate and badly broken shift symmetries, nor to identify a power counting parameter which suppresses the breaking.

Here, we will present explicit simple algebraic relations on the Wilson coefficients of the EFT Lagrangian in Eq. (6.1), which can be directly evaluated given a set of couplings and immediately yield an answer. These relations to be constructed below vanish iff the axion shift symmetry is preserved and whose size quantifies how badly it is broken, hence those quantities are order parameters of the breaking of the axion shift symmetry.

This is very similar in spirit to finding the Jarlskog invariant for CP violation in the SM, instead of scanning possible field redefinitions which absorb unphysical complex Lagrangian parameters, as discussed earlier. It may therefore not come as a surprise that our conditions are expressed in terms of flavour invariants, namely combinations of Lagrangian parameters which are left unchanged under fermion field redefinitions in flavour space. This allows us to encode the physical collective effects associated to the presence or absence of the axion shift symmetry.

Beyond explicit axion couplings to fermions, the CP-even axion-gauge bosons couplings are also flavourful when the PQ and the gauge symmetries have mixed anomalies. They do not break the shift symmetry at the perturbative level, but the gluon coupling does so at the non-perturbative level, as is crucial in QCD axion solutions to the strong CP problem. Therefore, we also study the order parameter for this non-perturbative breaking.

6.2 Flavour-Invariant Order Parameters for the Breaking of an Axion Shift Symmetry

We will approach the problem laid out in the previous section by asking the question under which condition the couplings $\tilde{Y}_{u,d,e}$ in the Yukawa basis of the ALP to the SM fields describe the couplings of a shift-symmetric axion. Furthermore, we want to identify the parameters, which break the shift symmetry and formulate them in terms of flavour-invariant order parameters of shift symmetry breaking.

We will start from the well-known relations derived earlier in Eq. (2.78)[2]

$$\exists C_{Q,u,d,L,e} \text{ hermitian, such that: } \tilde{Y}_{u,d} = i(Y_{u,d}C_{u,d} - C_Q Y_{u,d}) \ , \quad \tilde{Y}_e = i(Y_e C_e - C_L Y_e) \ . \tag{6.4}$$

However, these conditions are implicit, as they require a scan over all hermitian matrices $C_{Q,u,d,L,e}$. Therefore, it is an extremely hard task for a given set of $\tilde{Y}$ and SM Yukawa couplings to identify specific entries of the couplings matrices as the parameters breaking the axion shift symmetry, which should be sent to zero in order to recover the symmetry exactly.

Instead, we find it useful to deal with a set of algebraic conditions on $\tilde{Y}_{u,d,e}$ encoding the same information as the relations in Eq. (6.4) but do not implicitly depend on other unknown matrices C_ψ. In this section, we thus identify explicit, independent, necessary and sufficient conditions on the entries of $\tilde{Y}_{u,d,e}$ in Eq. (6.1) for the axion shift symmetry to hold. We focus on the experimentally relevant flavourful couplings of the SM, where all quark and lepton masses are non-vanishing and non-degenerate and where no texture zeros appear in the CKM matrix. Throughout most of this analysis, we neglect neutrino masses but will briefly comment on non-zero neutrino masses later in Sec. 6.3.2.

In some parts of this analysis, it can be useful to work in a specific flavour basis for the SM Yukawa couplings, for which we choose the following convention

$$Y_u = \text{diag}(y_u, y_c, y_t) \ , \quad Y_d = V_{\text{CKM}} \cdot \text{diag}(y_d, y_s, y_b) \ , \quad Y_e = \text{diag}(y_e, y_\mu, y_\tau) \ . \tag{6.5}$$

From this basis the mass basis can be reached by performing the field redefinition $d_L \to V_{\text{CKM}} d_L$.

Before we start constructing the order parameters for shift breaking, we want to remind the

[2]Note, that shift symmetry correlates the coupling of operators at higher order in $1/f$ couplings involving several axion fields and the same operator at $1/f$ with only one axion field. We will study this systematically using the Hilbert series in Chap. 7.

reader that the axion-dependent field redefinition translating between the bases in Eq. (6.3) and Eq. (6.1) also introduces shifts between the axion couplings to gauge fields [212] due to the mixed anomalies with the gauge group of the SM. These shifts depend on flavourful couplings and hence, can be naturally expressed using flavour invariants. The gluon coupling is particularly interesting, as it is a main driver of axion shift breaking in the regime of non-perturbative QCD. In the following, we will first focus on the fermionic couplings of the axion, but will come back to the gluon coupling in Sec. 6.5.

6.2.1 Parameter Counting with and without a Shift Symmetry

To set our expectations before starting with the construction of the relations on $\tilde{Y}_{u,d,e}$, we will fist do a counting of the number of relations that we expect by comparing the free parameters in the operator bases of Eq. (6.3) and Eq. (6.1), that are irremovable by fields redefinitions. It is helpful to count parameters separately according to their behaviour under the CP transformations introduced in Eq. (2.4). Since the axion is a pseudoscalar (i.e. it receives an additional sign w.r.t. the scalar in Eq. (2.4)), real $\tilde{Y}_\psi$ in Eq. (6.1) and imaginary C_ψ in Eq. (6.3) correspond to CP-odd couplings in the mass basis.

In the case of an explicitly broken shift symmetry, the EFT in the Yukawa basis of Eq. (6.1) should be used, where the couplings $\tilde{Y}$ are arbitrary complex 3×3 matrices. However, not all of the parameters in these matrices are physical because the presence of the lepton family numbers $U(1)_{L_i}$ as exact symmetries in the SM can be used to remove two phases among those of $\tilde{Y}_{e,i\neq j}$. Instead, the independent rephasing-invariant quantities are $\tilde{Y}_{e,ii}$, $\arg(\tilde{Y}_{e,ij}\tilde{Y}_{e,ji})$ $(i<j)$, $|\tilde{Y}_{e,ij}|$ and $\arg(\tilde{Y}_{e,12}\tilde{Y}_{e,23}\tilde{Y}_{e,31})$. In total, they yield 16 independent quantities, 7 CP-odd and 9 CP-even. In the quark sector, the baryon number rephasings, which are an exact symmetry in the SM, also leave the couplings of the effective operators invariant. Hence, all parameters in the quark sector of the EFT in Eq. (6.1) are physical and one finds $2 \times 9 = 18$ CP-even and $2 \times 9 = 18$ CP-odd couplings in the quark sector.

When the shift-symmetry is exact, we can work in the derivative basis of Eq. (6.3), where 2 hermitian matrices $C_{L,e}$ in the lepton sector and 3 hermitian matrices $C_{Q,u,d}$ in the quark sector parameterise all couplings of the axion to fermions. The lepton number rephasings can once more be used to remove two of the off-diagonal phases.[3] As discussed in Sec. 2.4.3, operators of the form $\partial_\mu a J^\mu$ in the derivative basis, for any conserved fermionic current of the SM J^μ, can be traded for couplings of the axion to the SM gauge fields $aX\tilde{X}$. Hence, the baryon and lepton family numbers of the SM, allow to remove one diagonal entry of either C_Q, C_u and three out of $C_{L,e}$. In total, there are 9 CP-even and 4 CP-odd couplings in the lepton sector, as well as 17 CP-even and 9 CP-odd couplings in the quark sector.

Comparing the counting in the two Lagrangians, we expect $7-4=3$ CP-odd relations and $9-9=0$ CP-even relations in the lepton sector together with $18-9=9$ CP-odd relations and $18-17=1$ CP-even relation in the quark sector, that characterise the presence of a shift symmetry in the basis of Eq. (6.1). The different countings are summarised in Table 6.1.

[3] The rephasing-invariants now read $C_{L/e,ii}, |c_{L/e,ij}|$ $(i<j)$, $\arg(C_{e,ij}C_{L,ji})$ $(i<j)$ and $\arg(C_{L,12}C_{L,23}C_{L,31})$.

	Shift-sym. WCs $C_{Q,u,d,L,e}$		Generic WCs $\tilde{Y}_{u,d,e}$		# constraints	
	CP-even	CP-odd	CP-even	CP-odd	CP-even	CP-odd
Quark sec.	17	9	18	18	1	9
Lepton sec.	9	4	9	7	0	3

Table 6.1: The number of physical coefficients at dimension 5 in the EFTs of Eq. (6.3) and Eq. (6.1), and numbers of constraints that $\tilde{Y}_{u,d,e}$ have to fulfil in order to respect an exact shift symmetry. A detailed counting can be found in the text.

6.2.2 Flavour Invariants in the Lepton Sector

We will now start deriving the relations, starting with the lepton sector, where the constraints turn out to be simpler than in the quark sector. We start from the matrix relation that maps the derivative basis to the Yukawa basis of the EFT

$$\tilde{Y}_e = i(Y_e C_e - C_L Y_e)\,. \tag{6.6}$$

For non-vanishing lepton masses, Y_e is invertible and one can solve the equation for C_e,

$$C_e = -iY_e^{-1}\left(\tilde{Y}_e + iC_L Y_e\right)\,. \tag{6.7}$$

Imposing that the anti-hermitian part $C_e^{(\mathrm{ah})} \sim C_e - C_e^\dagger$ of C_e vanishes leads to constraints, here expressed in the flavour basis of Eq. (6.5), where Y_e is diagonal and real

$$\exists C_L \text{ hermitian s.t. } \frac{\tilde{Y}_{e,ij}}{y_{e,i}} + \frac{\tilde{Y}^*_{e,ji}}{y_{e,j}} + iC_{L,ij}\left[\frac{y_{e,j}}{y_{e,i}} - \frac{y_{e,i}}{y_{e,j}}\right] = 0 \;\forall i,j\,. \tag{6.8}$$

When $i = j$, the second term vanishes and C_L disappears from the expression, revealing constraints only referring to the couplings $\tilde{Y}_e$, namely that $\tilde{Y}_{e,ii}$ is purely imaginary. The constraints imposed by Eq. (6.8) for $i < j$ and $i > j$ are complex conjugates of one another. Therefore we can analyse the two cases in one go by focusing on the case $i < j$, which can be solved by a suitable choice of C_L

$$C_{L,ii} = 0\,, \quad C_{L,ij,i<j} = i\frac{y_{e,j}\tilde{Y}_{e,ij} + y_{e,i}\tilde{Y}^*_{e,ji}}{y_{e,j}^2 - y_{e,i}^2}\,. \tag{6.9}$$

This simply defines a hermitian matrix C_L, bringing no further constraints. Therefore, Eq. (6.6) only imposes 3 conditions on $\tilde{Y}_e$ in order for it to describe a shift-symmetric axion, given that C_L, C_e are hermitian matrices. This is consistent with our previous counting of the free parameters in both EFT bases at the beginning of this section.

So far, we have only obtained the constraints in a specific flavour basis. However, it is an easy task to express the statement that the $\tilde{Y}_{e,ii}$ should be purely imaginary in a flavour-invariant way. By flavour invariant we mean here, that the relations are unchanged by the

	$SU(3)_Q$	$SU(3)_u$	$SU(3)_d$	$SU(3)_L$	$SU(3)_e$
$\tilde{Y}_u$	$\mathbf{3}$	$\bar{\mathbf{3}}$	$\mathbf{1}$	$\mathbf{1}$	$\mathbf{1}$
$\tilde{Y}_d$	$\mathbf{3}$	$\mathbf{1}$	$\bar{\mathbf{3}}$	$\mathbf{1}$	$\mathbf{1}$
$\tilde{Y}_e$	$\mathbf{1}$	$\mathbf{1}$	$\mathbf{1}$	$\mathbf{3}$	$\bar{\mathbf{3}}$

Table 6.2: Flavour transformation properties of the dimension-5 ALP Yukawa couplings treated as spurions under the flavour group. The SM Yukawa couplings transform similarly under $SU(3)^5$ and their behaviour under the transformations can be found in Tab. 2.2.

transformations of the flavour symmetry group, whose spurious action on the Lagrangian parameters of Eqs. (6.1) and (6.2) are given in Table 6.2. In the language of flavour invariants, the constraints on $\tilde{Y}_e$ read

$$\mathrm{Re}\,\mathrm{Tr}\Big(X_e^{0,1,2}\tilde{Y}_e Y_e^\dagger\Big) = 0 \ , \tag{6.10}$$

where we have defined $X_e \equiv Y_e Y_e^\dagger$. Later on, we will also repeatedly use $X_{u,d} \equiv Y_{u,d} Y_{u,d}^\dagger$. We want to stress again, that this quantity identifies the flavour-invariant, hence physical, order parameters of shift-symmetry breaking in the lepton sector.

6.2.3 Flavour Invariants in the Quark Sector

We will continue with the quark sector, where the presence of the left-handed quark doublet Q requires a simultaneous treatment of the up- and down-type quark couplings. The couplings $\tilde{Y}_{u,d}$ describe a shift-symmetric axion when

$$\exists C_{Q,u,d} \text{ hermitian s.t. } \tilde{Y}_{u,d} = i(Y_{u,d}C_{u,d} - C_Q Y_{u,d}) \ . \tag{6.11}$$

In analogy to the lepton case above, we can solve for $C_{u,d}$ when no mass vanishes. Imposing hermiticity of the matrices $C_{u,d}$ leads to the following constraints, once more expressed in the flavour basis of Eq. (6.5)

$$\exists c_Q \text{ hermitian s.t. } \begin{pmatrix} \dfrac{\tilde{Y}_{u,ij}}{y_{u,i}} + \dfrac{\tilde{Y}^*_{u,ji}}{y_{u,j}} + ic_{Q,ij}\left[\dfrac{y_{u,j}}{y_{u,i}} - \dfrac{y_{u,i}}{y_{u,j}}\right] \\ \dfrac{V^*_{\mathrm{CKM},ki}\tilde{Y}_{d,kj}}{y_{d,i}} + \dfrac{\tilde{Y}^*_{d,ki}V_{\mathrm{CKM},kj}}{y_{d,j}} + ic_{Q,kl}V^*_{\mathrm{CKM},ki}V_{\mathrm{CKM},lj}\left(\dfrac{y_{d,j}}{y_{d,i}} - \dfrac{y_{d,i}}{y_{d,j}}\right) \end{pmatrix} = 0 \ \forall i,j \ , \tag{6.12}$$

where we implicitly sum over k, l. As before, the dependence on the hermitian matrix C_Q corresponding to the left-handed field disappears in the $i = j$ equations. The implied constraints are identical to those found for the leptons and can be expressed in a flavour-invariant way as follows

$$\mathrm{Re}\,\mathrm{Tr}\Big(X_{u,d}^{0,1,2}\tilde{Y}_{u,d} Y_{u,d}^\dagger\Big) = 0 \ . \tag{6.13}$$

However, the presence of C_Q in the relations of both the up and down sector implies further conditions. They can be derived by first solving for the off-diagonal entries of C_Q using the relation involving $\tilde{Y}_u$,

$$C_{Q,ij,i<j} = i\frac{y_{u,j}\tilde{Y}_{u,ij} + y_{u,i}\tilde{Y}^*_{u,ji}}{y_{u,j}^2 - y_{u,i}^2}\,, \tag{6.14}$$

which can be inserted in the equations for $\tilde{Y}_d$ to obtain

$$\begin{aligned} &\frac{V^*_{\mathrm{CKM},ki}\tilde{Y}_{d,kj}}{y_{d,i}} + \frac{\tilde{Y}^*_{d,ki}V_{\mathrm{CKM},kj}}{y_{d,j}} \\ &+ i\sum_k\left[C_{Q,kk}V^*_{\mathrm{CKM},ki}V_{\mathrm{CKM},kj} + i\sum_{l\neq k}\frac{y_{u,l}\tilde{Y}_{u,kl} + y_{u,k}\tilde{Y}^*_{u,lk}}{y_{u,l}^2 - y_{u,k}^2}V^*_{\mathrm{CKM},ki}V_{\mathrm{CKM},lj}\right]\left(\frac{y_{d,j}}{y_{d,i}} - \frac{y_{d,i}}{y_{d,j}}\right) = 0 \end{aligned} \tag{6.15}$$

for $i < j$. For a generic CKM matrix, these three complex equations depend on two free real parameters, given by the differences $c_{Q,kk} - c_{Q,ll}$, and they yield four independent genuine constraints on $\tilde{Y}_{u,d}$. We would like to emphasise that these four conditions are *collective* effects, namely they only make sense when both the up- and down-type Yukawa couplings are present. We will illustrate this feature with explicit UV completions in Sec. 6.3.1. Together with the conditions in Eq. (6.13), we therefore find 10 conditions on the entries of $\tilde{Y}_{u,d}$ (consistently with our earlier counting), 4 of which entangle the up and down sectors.

It is difficult to write the remaining constraints in a flavour-invariant way, given the expressions we have found in the explicit flavour basis of Eq. (6.5). Therefore, we reconsider the matrix relations of Eq. (6.4) and will try to rewrite the relations we have just found in the specific flavour basis in a flavour-covariant form. The implicit relations for shift-symmetric axion Yukawa couplings

$$\tilde{Y}_{u,d} = i(Y_{u,d}C_{u,d} - C_Q Y_{u,d})\,, \tag{6.16}$$

can be solved for $C_{u,d}$ assuming that the quark Yukawa couplings are non-vanishing

$$C_{u,d} = -iY^{-1}_{u,d}\left(\tilde{Y}_{u,d} + iC_Q Y_{u,d}\right). \tag{6.17}$$

When the quark Yukawas $Y_{u,d}$ are full rank matrices, the vanishing of the anti-hermitian part of $C_{u,d}$ implies the following commutator relation

$$[c_Q, X_x] = i\left(\tilde{Y}_x Y_x^\dagger + Y_x\tilde{Y}_x^\dagger\right), \tag{6.18}$$

with $X_x = Y_x Y_x^\dagger$ and $x = u, d$. This commutator relation will be our main building block in constructing flavour invariants by exploiting well-known trace relations with commutators appearing in the traces. For instance, we can reproduce the constraints in Eq. (6.13) by using the fact that for any two matrices A, B

$$\mathrm{Tr}\left(A^n\left[A, B\right]\right) = 0 \quad \forall n \in \mathbb{Z}, \tag{6.19}$$

which implies

$$-i\,\mathrm{Tr}\left(X_x^n\left[c_Q, X_x\right]\right) = \mathrm{Tr}\left(X_x^n\left(\tilde{Y}_x Y_x^\dagger + Y_x\tilde{Y}_x^\dagger\right)\right) = 0 \tag{6.20}$$

For $x = u, d, e$ and $n = 0, 1, 2$, these equations correspond to the diagonal constraints we have found above. Additional trace identities presented in App. 6.A.1 enable us to derive more flavour invariants encoding the remaining conditions.

We want to quickly recapitulate what we have achieved so far. The matrix relations in Eq. (6.4) impose the presence of a shift symmetry on the generic couplings $\tilde{Y}_{u,d,e}$ in the effective interactions of a scalar a and the SM fermions. Hence, if these relations are imposed on the generic couplings, a shift symmetry for the axion will be present in the EFT. We have reformulated these conditions into a commutator relation in Eq. (6.18). Hence, if shift symmetry is imposed on the EFT, this commutation relation must hold true. Lastly, we managed to show using well-known trace relations, that if the commutator relations hold true, the trace of certain combinations of the SM Yukawa couplings $Y_{u,d,e}$ and the dimension-5 Yukawa couplings $\tilde{Y}_{u,d,e}$ must be zero. In summary, the 13 trace relations we have found are order parameters of shift symmetry breaking.

6.2.4 Complete Set of Linear Invariants

More trace relations can be used to construct flavour invariant quantities that encode the relation. To capture the relations encoding the shift symmetry of the ALP, as many independent trace relations with the corresponding behaviour under CP have to be found, as were counted in Sec. 6.2.1. Eventually, we consider the following set of flavour invariants, linear in $\tilde{Y}_{u,d,e}$

$$
\begin{aligned}
&I_u^{(1)} = \mathrm{Re\,Tr}\left(\tilde{Y}_u Y_u^\dagger\right), \qquad I_u^{(2)} = \mathrm{Re\,Tr}\left(X_u \tilde{Y}_u Y_u^\dagger\right), \qquad I_u^{(3)} = \mathrm{Re\,Tr}\left(X_u^2 \tilde{Y}_u Y_u^\dagger\right),\\
&I_d^{(1)} = \mathrm{Re\,Tr}\left(\tilde{Y}_d Y_d^\dagger\right), \qquad I_d^{(2)} = \mathrm{Re\,Tr}\left(X_d \tilde{Y}_d Y_d^\dagger\right), \qquad I_d^{(3)} = \mathrm{Re\,Tr}\left(X_d^2 \tilde{Y}_d Y_d^\dagger\right),\\
&I_{ud}^{(1)} = \mathrm{Re\,Tr}\left(X_d \tilde{Y}_u Y_u^\dagger + X_u \tilde{Y}_d Y_d^\dagger\right),\\
&I_{ud,u}^{(2)} = \mathrm{Re\,Tr}\left(X_u^2 \tilde{Y}_d Y_d^\dagger + \{X_u, X_d\} \tilde{Y}_u Y_u^\dagger\right),\\
&I_{ud,d}^{(2)} = \mathrm{Re\,Tr}\left(X_d^2 \tilde{Y}_u Y_u^\dagger + \{X_u, X_d\} \tilde{Y}_d Y_d^\dagger\right),\\
&I_{ud}^{(3)} = \mathrm{Re\,Tr}\left(X_d X_u X_d \tilde{Y}_u Y_u^\dagger + X_u X_d X_u \tilde{Y}_d Y_d^\dagger\right),\\
&I_{ud}^{(4)} = \mathrm{Im\,Tr}\left(\left[X_u, X_d\right]^2 \left(\left[X_d, \tilde{Y}_u Y_u^\dagger\right] - \left[X_u, \tilde{Y}_d Y_d^\dagger\right]\right)\right),
\end{aligned}
\tag{6.21}
$$

for the quarks and

$$
I_e^{(1)} = \mathrm{Re\,Tr}\left(\tilde{Y}_e Y_e^\dagger\right), \qquad I_e^{(2)} = \mathrm{Re\,Tr}\left(X_e \tilde{Y}_e Y_e^\dagger\right), \qquad I_e^{(3)} = \mathrm{Re\,Tr}\left(X_e^2 \tilde{Y}_e Y_e^\dagger\right) \tag{6.22}
$$

for the leptons. These invariants vanish if the EFT in the Yukawa basis describes a shift-symmetric ALP and their vanishing also provides a sufficient condition for the presence of a shift symmetry. To show this we take advantage of the linearity of the invariants in the dimension-5 Wilson coefficients $\tilde{Y}_{u,d,e}$ and use the transfer matrix introduced in Eq. (2.36). The rank of the transfer matrix, which amounts to the number of independent conditions associated with the set of equalities $I_A = 0 \; \forall A$ can be computed immediately from its defining equation and is found to be 13, 10 in the quark sector and 3 in the lepton sector. This is again in agreement with the counting performed in Sec. 6.2.1. Therefore, the invariants in Eqs. (6.21)-(6.22) vanish if and only if $\tilde{Y}_{u,d,e}$ describe the couplings of a shift-symmetric axion. We also want to stress again that they are algebraic and – unlike the complicated matrix relations in Eq. (6.4) – only depend on the Wilson coefficients in the Yukawa basis of the EFT. Hence, for a given set of values for the SM and effective ALP Yukawa couplings, evaluating the set of invariants is sufficient to discriminate between shift-invariant or shift-breaking couplings at the leading order in the EFT.

Note, that the set for the quark sector in Eq. (6.21) is not minimal as it contains the 11 invariants but only captures 10 independent conditions. Indeed, the invariants can be arranged into a vanishing linear combination, where the coefficients depend only on the SM flavour invariants derived in Sec. 2.5.1 of this thesis. Therefore, a subset of 10 non-redundant invariants can be found whose transfer matrix still has maximal rank. This is, for instance, achieved by the following set,

$$I_u^{(1)}, I_u^{(2)}, I_d^{(1)}, I_d^{(2)}, I_u^{(3)} + I_d^{(3)}, I_{ud}^{(1)}, I_{ud,u}^{(2)}, I_{ud,d}^{(2)}, I_{ud}^{(3)}, I_{ud}^{(4)} \,. \tag{6.23}$$

In the following we will still work with the redundant set as it is easier to show that the set is closed under RG flow by projecting onto a minimal set after performing the RG evolution.

Let us end this section by stressing that our conditions apply beyond the non-redundant operator basis of Eq. (6.1). In a redundant operator basis where both derivative coupled and operators from the Yukawa basis are present, our set of invariants still captures all sufficient and necessary conditions for the breaking of the ALP shift symmetry. This can be appreciated by using the linearity of the invariants in the Wilson coefficients. We can project the derivatively-coupled interactions onto the Yukawa basis and split the couplings into two parts

$$\tilde{Y} = \tilde{Y}^{(\mathrm{PQ})} + \tilde{Y}^{(\not{\mathrm{PQ}})} \,, \tag{6.24}$$

where the couplings induced by $\tilde{Y}^{(\mathrm{PQ})}$ respect a PQ symmetry and can therefore be written as in Eq. (6.3). Our set of invariants vanishes by construction on the $\tilde{Y}^{(\mathrm{PQ})}$, and, thanks to their linearity

$$I_A\left(\tilde{Y}\right) = I_A\left(\tilde{Y}^{(\not{\mathrm{PQ}})}\right) \,. \tag{6.25}$$

They therefore capture the sources of PQ breaking in the theory, irrespective of any shift-invariant couplings which are additionally present.

6.3 Examples and Properties

In this section, we illustrate the use of our invariants, highlight some of their properties, and comment on their connection to CP symmetry. More precisely, we confirm in Sec. 6.3.1 that our invariants capture the sources of shift symmetry breaking, as well as their collective nature, when the axion EFT is matched to UV models. We then connect in Sec. 6.3.2 our invariants to CP-odd invariants used in the study of CP violation, and we finally repeat in Sec. 6.3.3 the analysis in the low-energy EFT below the electroweak scale and in the EFT based on a non-linearly realised EW symmetry. The absence of weak interactions, which arrange left-handed (LH) up- and down-type quarks into a doublet, implies that the IR conditions are looser than those which hold in the EFT above the EW scale with more UV information.

6.3.1 Matching to UV Models

To illustrate some features of our invariants, we will match some simple flavourful axion models to the ALP EFT, confirming that the invariants capture the sources of PQ breaking and their collective nature. Here, we focus on shift-breaking perturbations of models which possess an exact PQ symmetry.

Axiflavon/Flaxion Model Let us start with the axiflavon/flaxion model [277–279] in which the Froggatt–Nielsen and Peccei–Quinn mechanisms are realised through the same spontaneously broken $U(1)$. In the model, a newly introduced complex scalar ϕ – the flavon – is subject to the following effective interactions with the SM fields[4]

$$-\mathcal{L} = \alpha_{ij}^{d}\left(\frac{\phi}{M}\right)^{q_{Q_i}-q_{d_j}} \bar{Q}_i H d_j + \alpha_{ij}^{u}\left(\frac{\phi}{M}\right)^{q_{Q_i}-q_{u_j}} \bar{Q}_i \tilde{H} u_j + \alpha_{ij}^{e}\left(\frac{\phi}{M}\right)^{q_{L_i}-q_{e_j}} \bar{L}_i H e_j + \text{h.c.} \quad (6.26)$$

with M the cut-off of the model and the $q_i \in \mathbb{R}$ are the charges of the SM fields under the $U(1)$, where a charge of +1 is assigned to the flavon and the Higgs is taken to be neutral. The symmetry is broken by the VEV $\langle\phi\rangle = f$ of the complex scalar, which in the model also determines the hierarchy of the SM Yukawa couplings. After spontaneous symmetry breaking, the flavon field can be linearly parameterised around its VEV $\phi = \frac{1}{\sqrt{2}}(f + s + ia)$ and the field a can be identified as the axion of the theory. Expanding the above Lagrangian in the unbroken electroweak phase we obtain for the interactions of the axion with the SM particles

$$-\mathcal{L} = \frac{ia}{f}\left(Y_{ij}^{d}\left(q_{Q_i} - q_{d_j}\right)\bar{Q}_i H d_j + Y_{ij}^{u}\left(q_{Q_i} - q_{u_j}\right)\bar{Q}_i \tilde{H} u_j + Y_{ij}^{e}\left(q_{L_i} - q_{e_j}\right)\bar{L}_i H e_j\right) + \text{h.c.} \quad (6.27)$$

where $Y_{ij}^{x} \equiv \alpha_{ij}^{x}\left(\frac{f}{\sqrt{2}M}\right)^{q_{x_{L,i}}-q_{x_{R,j}}}$ are the SM Yukawa couplings. The axion EFT couplings can simply be read off from this Lagrangian by comparing with Eq. (6.1)

$$\tilde{Y}_{u,ij} = iY_{ij}^{u}\left(q_{Q_i} - q_{u_j}\right), \quad \tilde{Y}_{d,ij} = iY_{ij}^{d}\left(q_{Q_i} - q_{d_j}\right), \quad \tilde{Y}_{e,ij} = iY_{ij}^{e}\left(q_{L_i} - q_{e_j}\right). \quad (6.28)$$

The Lagrangian in Eq. (6.26) is constructed to be Peccei-Quinn invariant, hence all couplings in Eq. (6.27) must correspond to a shift-symmetric axion.[5] This is consistent with the fact

[4] This effective Lagrangian can be UV-completed in a theory of vector-like fermions of mass M which couple to the SM fermions and ϕ [270, 280].

[5] Beyond the precise model discussed in this section, Eq. (6.27) describes any set of shift-symmetric axion couplings in the flavour basis which diagonalises the PQ symmetry, i.e. where it acts as a phase shift on each flavour independently. This basis is the one which diagonalises all couplings c in Eq. (6.3), which read $c_{\psi,ij} = -q_{\psi_i}\delta_{ij}$ for each fermion field ψ.

that our invariants I vanish when evaluated on the above couplings. For instance,

$$I_u^{(1)} = -\mathrm{Im}\,\mathrm{Tr}\left([\mathrm{diag}\,(q_Q)\,Y^u - Y^u\mathrm{diag}\,(q_u)]\,Y^{u\dagger}\right) = 0 \ , \tag{6.29}$$

due to the cyclicity of the trace and the fact that the imaginary part of the trace of a hermitian matrix vanishes. All other invariants in the set evaluated on the Wilson coefficients matched to the model vanish as well. The invariants become non-zero when a generic Peccei-Quinn breaking term is introduced

$$-\mathcal{L}_{\not{PQ}} = \epsilon\frac{ia}{f}\left(\beta^d_{ij}\bar{Q}_i H d_j + \beta^u_{ij}\bar{Q}_i\tilde{H}u_j + \beta^e_{ij}\bar{L}_i H e_j\right) + \text{h.c.} \tag{6.30}$$

which we give a generically different power counting ϵ than the Peccei-Quinn invariant Lagrangian (these couplings can originate from terms as in Eq. (6.26), but where the charged $q_{x_{L,i}} - q_{x_{R,j}} \to n^x_{ij}$ violate the PQ symmetry and $\alpha_x \to \epsilon\alpha'_x$). We can match this Lagrangian at tree level to the ALP EFT defined in Eq. (6.1), yielding

$$\tilde{Y}_{u,ij} = iY^u_{ij}\left(q_{Q_i} - q_{u_j}\right) + i\epsilon\beta^u_{ij}, \quad \tilde{Y}_{d,ij} = iY^d_{ij}\left(q_{Q_i} - q_{d_j}\right) + i\epsilon\beta^d_{ij}, \quad \tilde{Y}_{e,ij} = iY^e_{ij}\left(q_{L_i} - q_{e_j}\right) + i\epsilon\beta^e_{ij}. \tag{6.31}$$

Plugging this into our invariants I yields expressions of the form

$$\{I\}_{I\in\text{minimal set}} = \epsilon f_I(Y_{ij}, \beta_{ij}, q_i) \tag{6.32}$$

where the f_I are complicated polynomials of the parameters of the theory (the dependence in ϵ, β_{ij} and q_i is linear, due to the linearity of our invariants). It can easily be checked that taking the shift-symmetric limit $\epsilon \to 0$ makes all invariants vanish, as expected.

We can further confirm that our invariants act as order parameters of the ALP shift-symmetry and illustrate their features by considering more specific realisations of the PQ-breaking term. For instance, let us add to Eq. (6.26) the term

$$-\mathcal{L}_{\not{PQ}} = \delta_{i1}\delta_{j1}\alpha'\left(\frac{\phi}{M}\right)^{q'_{Q_i}-q'_{u_j}}\bar{Q}_i\tilde{H}u_j + \text{h.c.}\ . \tag{6.33}$$

This shifts the SM Yukawa and axion couplings with respect to those of the PQ-symmetric axiflavon model as follows

$$Y_{u,ij} \to Y_{u,ij} + y'\delta_{i1}\delta_{j1}\ , \quad \tilde{Y}_{u,ij} \to \tilde{Y}_{u,ij} + i(q'_{Q_i} - q'_{u_j})y'\delta_{i1}\delta_{j1}\ , \tag{6.34}$$

with $y' \equiv \left(\frac{f}{\sqrt{2}M}\right)^{q'_{Q_1}-q'_{u_1}}\alpha'$, hence

$$\beta_{u,ij} = (q'_{Q_i} - q'_{u_j} - [q_{Q_i} - q_{u_j}])y'\delta_{i1}\delta_{j1}\ , \tag{6.35}$$

in the language of Eq. (6.30). Then, one finds that all our invariants are proportional to the one quantity which violates the PQ symmetry, namely $q_{Q_1} - q_{u_1} - \left[q'_{Q_1} - q'_{u_1}\right]$. For instance,

$$I_u^{(1)} = \left(q_{Q_1} - q_{u_1} - \left[q'_{Q_1} - q'_{u_1}\right]\right) \mathrm{Im}\left(y' Y^{u\,*}_{11}\right) \ . \tag{6.36}$$

From this expression it is clear, that the invariants are exactly zero when the PQ symmetry is restored and deviate from it proportionally to the spurion which breaks the symmetry.

The collective nature of shift-breaking effects in the EFT can be illustrated well by considering the couplings in Eq. (6.26), where we add a term to the Lagrangian such that we modify $q_{Q_1} \to q'_{Q_1}$ only in the up-type quark coupling but not in the same coupling to the down-type quarks. In this case, the quantity $q'_{Q_1} - q_{Q_1}$ violates the PQ symmetry, but it is only resolved by invariants which are sensitive to the collective nature of PQ breaking, namely those which simultaneously involve $\tilde{Y}_u$ and $\tilde{Y}_d$. Indeed, the change $q_{Q_1} \to q'_{Q_1}$ is a mere relabelling from the perspective of the up-type quarks alone, but it breaks PQ when the down-type quarks are taken into account. Consistently, we have

$$I_u^{(1)} = -\mathrm{Im}\,\mathrm{Tr}\left(\left[\mathrm{diag}\left(q'_Q\right) Y^u - Y^u \mathrm{diag}\left(q_u\right)\right] Y^{u\dagger}\right) = 0 \ , \tag{6.37}$$

where $q'_{Q_j} \equiv q_{Q_j} + \delta_{j1}\left(q'_{Q_1} - q_{Q_1}\right)$, whereas for instance

$$I_{ud}^{(1)} = \frac{1}{2i}\left(q_{Q_1} - q'_{Q_1}\right)\left[X_u, X_d\right]_{11} \ . \tag{6.38}$$

Weinberg-Wilczek Model Another class of UV models that can embed an axion are two-Higgs-doublet models (2HDM) (see e.g. [281] for a review), like the WW model we have introduced in Sec. 2.4.2. For definiteness, we consider the WW model with a 2HDM of type II with the following PQ-preserving Lagrangian in the quark sector

$$-\mathcal{L} = \bar{Q} Y_u^{(1)} \tilde{H}_1 u + \bar{Q} Y_d^{(2)} H_2 d + \mathrm{h.c.}\,. \tag{6.39}$$

The scalar potential is chosen to be invariant under a global $U(1)$ PQ symmetry. This fixes the PQ charges q_{H_i} of the Higgses up to a global normalisation. The non-vanishing difference $q_{H_1} - q_{H_2}$ allows us to introduce PQ-breaking in the Yukawa sector, as we will see below.

After integrating out the massive Higgses as well as removing the gauge Goldstone bosons, one can describe the axion couplings as well as the fermion mass terms by the replacement

$$H_i = e^{i q_{H_i} \frac{a}{f}} \frac{v_i}{v} H \ , \ \text{with } H = \begin{pmatrix} 0 \\ \frac{v}{\sqrt{2}} \end{pmatrix} \ , \ v^2 \equiv v_1^2 + v_2^2 \ . \tag{6.40}$$

As discussed in Sec. 2.4.2, the PQ-breaking scale can be decoupled from the EW scale by introducing another scalar as is done in DFSZ-like models. Here, we work with a WW-type model to simplify the illustration of properties of the invariants. The replacement of the Higgs with the remaining angular excitation around its VEV reproduces the appropriate PQ transformations, $H_i \xrightarrow{\mathrm{PQ}} e^{i\alpha_{\mathrm{PQ}} q_{H_i}} H_i$ for α_{PQ} the transformation parameter, since $a \xrightarrow{\mathrm{PQ}}$

$a + 2\pi\alpha_{\text{PQ}} f$. We find as expected that our invariants vanish, when they are evaluated on the Wilson coefficients subject to the following matching expressions

$$Y_u = \frac{v_1}{v} Y_u^{(1)} , \quad Y_d = \frac{v_2}{v} Y_d^{(2)} , \quad \tilde{Y}_u = -i q_{H_1} Y_u , \quad \tilde{Y}_d = i q_{H_2} Y_d . \tag{6.41}$$

The Lagrangian can be amended in a way where it breaks the PQ symmetry, highlighting different aspects of our invariants. Starting with

$$-\mathcal{L}_{\not{P}\not{Q}} = Y_{u,ij}^{(2)} \bar{Q}_i \tilde{H}_2 u_j + \text{h.c. with } Y_{u,ij}^{(2)} = \delta_{i1}\delta_{j1} Y_{u,11}^{(2)} , \tag{6.42}$$

the Yukawa and axion couplings of the PQ-preserving Lagrangian are shifted as

$$Y_u = \frac{v_1}{v} Y_u^{(1)} + \frac{v_2}{v} Y_u^{(2)} , \quad \tilde{Y}_u = -i q_{H_1} \frac{v_1}{v} Y_u^{(1)} - i q_{H_2} \frac{v_2}{v} Y_u^{(2)} . \tag{6.43}$$

The invariants featuring only up-type couplings are then proportional to real/imaginary parts of $(q_{H_1} - q_{H_2}) Y_{u,11}^{(2)}$, as expected given the different ways to obtain an exact PQ symmetry in this sector (for a generic $Y_u^{(1)}$). We find, for instance

$$I_u^{(1)} = (q_{H_1} - q_{H_2}) \frac{v_1 v_2}{v^2} \text{Im Tr} \left(Y_u^{(2)} Y_u^{(1)\dagger} \right) = -(q_{H_1} - q_{H_2}) \frac{v_1 v_2}{v^2} \text{Im} \left(Y_{u,11}^{(2)} Y_{u,11}^{(1)\,*} \right) . \tag{6.44}$$

As in the Froggatt–Nielsen case, we can illustrate the collective nature of the shift symmetry. To show this let us further assume that $Y_{u,1j}^{(1)} = 0$, which is such that the up-type quark couplings do not violate the PQ symmetry until the down-type quarks are taken into account. Indeed, we find

$$I_u^{(1)} = 0 , \tag{6.45}$$

whereas, for instance, one of the invariants including both up- and down-type couplings evaluates to

$$I_{ud}^{(1)} = -\frac{1}{2i} \left(q_{H_1} - q_{H_2} \right) \frac{v_1 v_2}{v^2} \left[X_u, X_d \right]_{11} . \tag{6.46}$$

Weakly Broken PQ Symmetry Let us close by making a general statement for any model with an approximate PQ symmetry, characterised by a small breaking parameter ϵ: the invariants of Eqs. (6.21)-(6.22) are all ϵ-suppressed. This follows from the linearity of our invariants emphasised at the end of section 6.2.4. Indeed, in models with a weakly-broken PQ symmetry, the Yukawa couplings are split into

$$\tilde{Y} = \tilde{Y}^{(\text{PQ})} + \tilde{Y}^{(\not{P}\not{Q})} , \tag{6.47}$$

where $\tilde{Y}^{(\not{P}\not{Q})} = \mathcal{O}(\epsilon)$ and $\tilde{Y}^{(\text{PQ})}$ respects an exact axion shift symmetry, i.e. our invariants vanish when evaluated on $\tilde{Y}^{(\text{PQ})}$. Due to the linearity of the invariants, they are suppressed by ϵ as claimed.

6.3.2 Connection to CP Violation

The possibility to reintroduce CP violation through the axion, which is constructed to solve the strong CP problem, has mostly been disregarded in the literature and has only gained more attention recently [189, 282–288] (for a recent review see Ref. [289]). There is a close interplay between leading order CP violation and shift symmetry in the ALP Lagrangian. Adapting the results of Ref. [103], we find the following necessary and sufficient conditions for CP to be conserved in the quark sector of the Yukawa basis of the ALP EFT

$$\begin{aligned} J_4 &= L_{0000}(\tilde{Y}_x Y_x^\dagger) = L_{1000}(\tilde{Y}_x Y_x^\dagger) = L_{0100}(\tilde{Y}_x Y_x^\dagger) \\ &= L_{1100}(\tilde{Y}_x Y_x^\dagger) = L_{0110}(\tilde{Y}_x Y_x^\dagger) = L_{2200}(\tilde{Y}_x Y_x^\dagger) \\ &= L_{0220}(\tilde{Y}_x Y_x^\dagger) = L_{1220}(\tilde{Y}_x Y_x^\dagger) = L_{0122}(\tilde{Y}_x Y_x^\dagger) = 0 \end{aligned} \tag{6.48}$$

with $L_{abcd}(\tilde{C}) \equiv \mathrm{Re}\,\mathrm{Tr}\left(X_u^a X_d^b X_u^c X_d^d \tilde{C}\right)$, $x = u, d$ and J_4 is the Jarlskog invariant, capturing all perturbative CP violation in the SM. If this is compared with our set of shift symmetry invariants in Eq. (6.21), we find that all invariants but $I_{ud}^{(4)}$ can be expressed as combinations of the CP-odd invariants. For instance, $I_u^{(1)} = L_{0000}(\tilde{Y}_u^\dagger Y_u)$ and $I_{ud}^{(1)} = L_{0100}(\tilde{Y}_u^\dagger Y_u) + L_{1000}(\tilde{Y}_d^\dagger Y_d)$. Therefore, most sources of leading order shift-breaking in the ALP EFT also source CP violation, hence CP conservation almost implies axion shift symmetry. This connection is only spoilt by $I_{ud}^{(4)}$, namely the one CP-even shift-symmetric invariant of our set that has to be included in order to obtain a full rank transfer matrix. Furthermore, the connection holds exactly in the lepton sector of the EFT.

In the degenerate cases, where the flavour symmetry of the SM is enlarged with respect to $U(1)_B \times U(1)_{L_i}$, CP conservation implies shift invariance at the level of the coefficients which can interfere with the dimension-four coefficients, i.e. at the level of observables computed at $\mathcal{O}(1/f)$. It is however not sufficient for observables computed beyond that order. See Ref. [1] for more details.

Conversely, an exact shift symmetry also correlates sources of CP violation in the axion EFT. E.g., requiring that $I_{ud}^{(1)}$ vanishes implies that $L_{0100}(\tilde{Y}_u^\dagger Y_u) = -L_{1000}(\tilde{Y}_d^\dagger Y_d)$. These correlations, that emerge from the collectiveness of shift breaking, have an impact on CP-violating observables like EDMs and allow us to relate the contributions of up- and down-type quarks to those observables. If a sufficient amount of data from CP violating observables is available to constrain all parameters in the quark sector, these correlations would allow us to distinguish a shift symmetric ALP, for which the correlations are present, from a non-shift symmetric ALP. We will study the implications of axion shift invariance on EDMs in Sec. 6.4.2.

It is also interesting to understand why there are exactly 9 CP-odd and 1 CP-even parameters which capture the shift-breaking interactions in the quark sector of the ALP EFT at the leading order. One can first notice that this is exactly the same number of parameters as there are physical parameters in the quark sector of the renormalisable Lagrangian (captured by the flavour invariants presented in Eq. (2.98)), but with opposite CP parity due to the ALP being a pseudoscalar.

This is true as well in the much simpler lepton sector, but also holds true for more complicated theories with more fermions coupled to the ALP. Let us briefly demonstrate this with the example of sterile neutrinos added to the SM, both with a Yukawa coupling and a Majorana mass term, as we studied earlier in Chaps. 3 and 4. For instance, adding 3 generations of sterile neutrinos to the EFT, yields 9 masses, 6 mixing angles and 6 phases, i.e. 15 CP-even and 6 CP-odd physical parameters in the lepton sector of the renormalisable theory (see e.g. Ref. [261]). The light sterile neutrinos N also have to be added to the particle spectrum considered in the construction of the EFT. The EFT Lagrangian in the lepton sector in the derivatively coupled basis has the following form

$$\mathcal{L} \supset \frac{\partial_\mu a}{f}\bar{L}C_L\gamma^\mu L + \frac{\partial_\mu a}{f}\bar{e}C_e\gamma^\mu e + \frac{\partial_\mu a}{f}\bar{N}C_N\gamma^\mu N\,. \tag{6.49}$$

After performing an ALP-dependent field redefinition, we can also switch to the Yukawa basis

$$\mathcal{L} \supset \frac{a}{f}\left(\bar{L}\tilde{Y}_e He + \bar{L}\tilde{Y}_N HN + \bar{N}^c\tilde{M}_N N + \text{h.c.}\right)\,. \tag{6.50}$$

As discussed before, one can impose relations on the couplings of the second Lagrangian such that it captures the same physics as the first Lagrangian. We will not construct them explicitly here, but will just count the number of physical parameters in both Lagrangians to obtain the number of relations that have to be imposed, as we have also done for all other couplings in Sec. 6.2.1. The first Lagrangian has 3 hermitian coupling matrices C_e, C_L, C_N, i.e. 3×6 CP-even and 3×3 CP-odd couplings. Because the Majorana mass term $\bar{N}^c M_N N$ of the sterile neutrinos breaks lepton (family) number, there are no conditions of the form $\partial_\mu j^\mu = 0$ that have to be imposed. The second Lagrangian has 2 generic coupling matrices $\tilde{Y}_e, \tilde{Y}_N$ with 2×9 CP-even and 2×9 CP-odd parameters, while the symmetric coupling $\tilde{M}_N$ has 6 CP-even and 6 CP-odd couplings. Again, because lepton (family) number is broken, no rephasings are allowed and all couplings remain physical. Comparing the two EFTs, we find a discrepancy of 6 CP-even and 15 CP-odd couplings which exactly corresponds to the number of physical parameters in the renormalisable Lagrangian of the theory with opposite CP parity.

This correspondence between the number of physical parameters in the renormalisable Lagrangian and the number of shift-breaking parameters in the leading interactions of the ALP EFT can be understood by considering the field redefinitions that make the ALP EFT in the Yukawa basis shift-invariant [213]. A shift of the ALP $a \to a + c$ in the Yukawa basis of the EFT can be removed by performing a flavourful field redefinition $\psi \to c_\psi \frac{c}{f}\psi$. The field redefinition redefines the SM Yukawa in such a way, that it will force the Wilson coefficients to be exactly of the form of Eq. (6.4). Therefore, for each physical parameter present in the Yukawa couplings at dimension 4, one has the freedom to remove a parameter at dimension 5. Furthermore, if there is a degeneracy in the mass spectrum at dimension 4 that increases the exact flavour group of the renormalisable Lagrangian, one also has more freedom to remove parameters at dimension-5, preserving this correspondence even for degenerate spectra. This however does not mean that if CP conservation is imposed at dimension-4 that the single CP-even shift-breaking coupling at dimension 5 will automatically vanish. The parameters at dimension 4 only enter a relation with the dimension-5 parameters by the field redefinition and the same behaviour under flavour transformations. It is exactly this behaviour under flavour transformations that allows us to remove more parameters in the case of a degenerate spectrum at dimension 4. Setting the phase of the CKM matrix to zero does not increase the flavour symmetry and therefore the independent parameter at dimension 5 cannot be removed.

Therefore, imposing CP conservation on the EFT with shift-breaking operators does not yield a shift-symmetric EFT as one might expect. This can be seen in a straightforward way from the invariants in Eqs. (6.21) and (6.22). The real and imaginary part of the invariant immediately indicate the behaviour of the given constraint under CP.

Note that this correspondence only holds for the leading order interactions that are of the same form as the corresponding mass term that is exploited to remove the shift-breaking terms by the use of field redefinitions. We will explicitly study these higher order interactions in Chap. 7.

6.3.3 Shift Invariance Below the Electroweak Scale or for a Non-Linearly Realised Electroweak Symmetry

As we have seen throughout this chapter both in the construction of the invariants and their matching to UV completions, the conditions for shift symmetry are affected by gauge interactions. Indeed, the presence of electroweak interactions generated entangled conditions in the quark sector. Therefore, it is interesting to run the same analysis in the low-energy EFT below the electroweak scale, where the heavy particles of the SM, the W, Z, h bosons and the top quark t are integrated out.[6]

Below the scale of electroweak symmetry breaking, the gauge interactions reduce to those of electromagnetism and QCD, and the mass terms in the dimension-4 Lagrangian reads as follows

$$\mathcal{L} \supset -\bar{u}_L m_u u_R - \bar{d}_L m_d d_R - \bar{e}_L m_e e_R + h.c. \ , \tag{6.51}$$

where $m_{u,d,e}$ are $(2\times 2, 3\times 3$ and $3\times 3)$ complex matrices. The derivatively coupled dimension-five couplings to the axion are identical to those of Eq. (6.3), except that now $\psi \in \{(u,d,e)_{L,R}\}$. The couplings of a generic pseudoscalar to the fermions read

$$\mathcal{L} \supset -\frac{a}{f}\left(\bar{u}_L \tilde{m}_u u_R + \bar{d}_L \tilde{m}_d d_R + \bar{e}_L \tilde{m}_e e_R + h.c.\right) \ , \tag{6.52}$$

in analogy to Eq. (6.1), with the notable difference that the up- and down-type quark sectors are decoupled. Due to this decoupling, entangled relations like those in the quark sector in the EFT above the EW scale no longer exist, because the left-handed quarks are no longer forced into an $SU(2)$ doublet. Following our previous analysis, it follows immediately that all conditions encoding the shift symmetry come in the form of those in the lepton sector of

[6] Our discussion also applies to the EFT, where the top quark is kept in the theory, as long as no electroweak couplings contribute. In that case, all matrices remain 3×3 complex matrices in flavour space.

the EFT above the EW scale

$$I_x^{(i+1,\mathrm{IR})} \equiv \mathrm{Tr}\Big(X_x^{i=0,1,\ldots,N_x-1}\tilde{m}_x m_x^\dagger\Big) = 0\ , \tag{6.53}$$

where $x = u, d, e$, $N_u = 2, N_{d,e} = 3$ and here $X_x \equiv m_x m_x^\dagger$.

The number of constraints in the IR reduces with respect to that in the UV because there are no longer conditions connecting the up- and down-sectors. This is not very surprising because we have derived the UV conditions under the assumptions that the axion couples to the degrees of freedom of the SM, which linearly realise the EW symmetry $SU(2)_L \times U(1)_Y$. However, the most general UV resolution of $SU(2)_L \times U(1)_Y$ may need to be phrased using the language of non-linear realisations of symmetries [173, 174], which can be applied to the EW symmetry [84] and its extension to axion couplings [194]. In the case of a non-linearly realised EW symmetry, the Goldstone bosons which generate the longitudinal components of massive W and Z bosons have to be treated independently of the physical Higgs h. Using the CCWZ construction, one conveniently packages the Goldstone boson multiplet π^a of the spontaneously broken symmetry into a matrix U as follows

$$U = e^{i\pi^a\sigma^a/v}\ , \tag{6.54}$$

where σ^a are the Pauli matrices and v is the EW VEV. U has convenient transformations under $SU(2)_L \times U(1)_Y$,

$$U \to e^{i(\alpha_Y + \alpha^a\sigma^a/2)}U\ , \tag{6.55}$$

and the physical Higgs scalar h is independently added to the theory as a gauge singlet. The usual linear realisation can be recovered by defining

$$H = U\begin{pmatrix} 0 \\ \frac{v+h}{\sqrt{2}} \end{pmatrix}\ , \tag{6.56}$$

and using H only to write couplings.

When U and h are treated independently, as it is the case for non-linear realisations, one can supplement the Lagrangian of Eq. (6.3) by additional shift-invariant fermionic operators at dimension five (see [194] for a complete treatment)

$$\frac{\partial_\mu a}{f}\sum_{\psi=Q,L}\bar{\psi}\tilde{c}_\psi T\gamma^\mu\psi\ , \quad T \equiv U\sigma_3 U^\dagger\ . \tag{6.57}$$

By working in unitary gauge where $U = \mathbb{1}$, it is clear that these operators allow one to decorrelate the couplings of the different components of an $SU(2)_L$ doublet. The axion-fermion couplings of the generic basis of Eq. (6.1) now map to

$$\frac{a}{f}\left(\bar{Q}_L U\left[K_Q + \sigma_3\tilde{K}_Q\right]\begin{pmatrix} u_R \\ d_R \end{pmatrix} + \bar{L}_L U\left[K_L + \sigma_3\tilde{K}_L\right]\begin{pmatrix} 0 \\ e_R \end{pmatrix}\right)\ . \tag{6.58}$$

While more structures can be added in the derivatively coupled basis of the EFT in the scenario of a non-linearly realised EW symmetry, the number of building blocks for the invariants is unchanged with respect to Eq. (6.1). This is easily seen by identifying

$$\tilde{Y}_{u,d} = K_Q \pm \tilde{K}_Q \;, \quad \tilde{Y}_e = K_L - \tilde{K}_L \,. \tag{6.59}$$

Therefore, the conditions to be shift-invariant in a non-linear realisation of the EW symmetry correspond to three copies (for u, d, e) of the lepton conditions of Eq. (6.10).

Since a pure IR study of the shift invariance property has to capture both of these scenarios, it cannot reproduce more than three copies of lepton-like conditions. Nevertheless, assuming a matching to a linear phase of the EW symmetry and an exact axion shift symmetry, we will show in section 6.4.2 that more conditions remain valid at leading order under the RG flow.

6.4 Renormalisation Group Evolution

In previous sections, we presented flavour-invariant order parameters for the breaking of the axion shift symmetry. As any complete set of order parameters, it should be closed under the RG flow which preserves symmetries of the Lagrangian[7]. This is what we show in section 6.4.1. In section 6.4.2, we descend to the IR EFT below the electroweak scale and find that the relations inherited from the UV under tree-level matching are maintained by the RG running below the electroweak scale, although they do not strictly follow from shift symmetry in the IR. We also revisit EDM bounds on CP-violating axion couplings under the assumption of an approximate shift symmetry. Finally, in section 6.4.3 we illustrate the use of our invariants by working out sum rules on the axion-induced RG running of SMEFT operators at dimension-six.

6.4.1 Renormalisation Group Running Above the Electroweak Scale

To verify the completeness of our set of invariants, we can calculate their RG evolution under which the set should be closed. Using the RGEs of the components [212, 213] of the invariants yields for the lepton invariants

$$\begin{aligned}
\dot{I}_e^{(1)} &= 2\gamma_e I_e^{(1)} + 6 I_e^{(2)} + 2\,\mathrm{Tr}(X_e)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_e^{(2)} &= 4\gamma_e I_e^{(2)} + 9 I_e^{(3)} + 2\,\mathrm{Tr}\!\left(X_e^2\right)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_e^{(3)} &= 6\gamma_e I_e^{(3)} + 12 I_e^{(4)} + 2\,\mathrm{Tr}\!\left(X_e^3\right)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right)
\end{aligned} \tag{6.60}$$

where $\dot{I} = 16\pi^2 \mu \frac{dI}{d\mu}$ and we have introduced a short notation for the wave function renormalisation $\gamma_e = -\frac{15}{4} g_1^2 - \frac{9}{4} g_2^2 + \mathrm{Tr}\left(X_e + 3(X_u + X_d)\right)$, which appears in a generic manner in all RGEs.

[7] This is for instance the case for the flavour invariants of the quark sector [290] of the SM and the lepton sector of the SM with Majorana neutrino masses [220, 253].

The invariant $I_e^{(4)} = \mathrm{Re}\,\mathrm{Tr}\left(X_e^3 \tilde{Y}_e Y_e^\dagger\right)$ appearing in the RGE of $I_e^{(3)}$ is not independent of the invariants in Eq. (6.22), since due to the Cayley-Hamilton theorem the nth power of any $n \times n$ matrix can be can be expressed in terms of lower powers and traces of lower powers of the matrix. For a 3×3 matrix A, the Cayley-Hamilton theorem has the form [218]

$$A^3 = A^2\,\mathrm{Tr}\,A - \frac{1}{2} A\left((\mathrm{Tr}\,A)^2 - \mathrm{Tr}\,A^2\right) + \frac{1}{6}\mathbb{1}\left((\mathrm{Tr}\,A)^3 - 3\,\mathrm{Tr}\,A^2\,\mathrm{Tr}\,A + 2\,\mathrm{Tr}\,A^3\right), \tag{6.61}$$

which allows us to reexpress $I_e^{(4)}$ as follows

$$I_e^{(4)} = \mathrm{Tr}(X_e) I_e^{(3)} - \frac{1}{2}\left((\mathrm{Tr}\,X_e)^2 - \mathrm{Tr}\,X_e^2\right) I_e^{(2)} + \frac{1}{6}\left((\mathrm{Tr}\,X_e)^3 - 3\ \mathrm{Tr}\,X_e^2\,\mathrm{Tr}\,X_e + 2\,\mathrm{Tr}\,X_e^3\right) I_e^{(1)}. \tag{6.62}$$

Therefore, the set of RGEs in Eq. (6.60) does indeed form a closed set of differential equations and hence the set of lepton invariants in Eq.(6.22) is complete.

For the quark sector we find the following set of RGEs

$$\begin{aligned}
\dot{I}_u^{(1)} &= 2\gamma_u I_u^{(1)} + 6 I_u^{(2)} - 3 I_{ud}^{(1)} - 2\,\mathrm{Tr}(X_u)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_u^{(2)} &= 4\gamma_u I_u^{(2)} + 9 I_u^{(3)} - 3 I_{ud,u}^{(2)} - 2\,\mathrm{Tr}\left(X_u^2\right)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_u^{(3)} &= 6\gamma_u I_u^{(3)} + 12 I_u^{(4)} - 3 I_u' - 2\,\mathrm{Tr}\left(X_u^3\right)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_d^{(1)} &= 2\gamma_d I_d^{(1)} + 6 I_d^{(2)} - 3 I_{ud}^{(1)} + 2\,\mathrm{Tr}(X_d)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_d^{(2)} &= 4\gamma_d I_d^{(2)} + 9 I_d^{(3)} - 3 I_{ud,d}^{(2)} + 2\,\mathrm{Tr}\left(X_d^2\right)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_d^{(3)} &= 6\gamma_d I_d^{(3)} + 12 I_d^{(4)} - 3 I_d' + 2\,\mathrm{Tr}\left(X_d^3\right)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_{ud}^{(1)} &= 2(\gamma_u + \gamma_d) I_{ud}^{(1)}, \\
\dot{I}_{ud,u}^{(2)} &= (4\gamma_u + 2\gamma_d) I_{ud,u}^{(2)} + 3 I_u' - 6 I_{ud}^{(3)} - 2\,\mathrm{Tr}(X_u X_d X_u)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_{ud,d}^{(2)} &= (4\gamma_d + 2\gamma_u) I_{ud,d}^{(2)} + 3 I_d' - 6 I_{ud}^{(3)} + 2\,\mathrm{Tr}(X_d X_u X_d)\left(I_e^{(1)} + 3(I_d^{(1)} - I_u^{(1)})\right), \\
\dot{I}_{ud}^{(3)} &= 4(\gamma_u + \gamma_d) I_{ud}^{(3)}, \\
\dot{I}_{ud}^{(4)} &= 6\left(\gamma_u + \gamma_d + \frac{1}{2}\mathrm{Tr}(X_u + X_d)\right) I_{ud}^{(4)} - \mathrm{Im}\,\mathrm{Tr}\left([X_u, X_d]^3\right)(I_u^{(1)} + I_d^{(1)}),
\end{aligned} \tag{6.63}$$

where we have again introduced a short notation for the wave function renormalisation $\gamma_u \equiv -\frac{17}{12}g_1^2 - \frac{9}{4}g_2^2 - 8g_3^2 + \mathrm{Tr}(X_e + 3(X_u + X_d))$ and $\gamma_d \equiv -\frac{5}{12}g_1^2 - \frac{9}{4}g_2^2 - 8g_3^2 + \mathrm{Tr}(X_e + 3(X_u + X_d))$.

The invariants $I_u^{(4)}, I_d^{(4)}$ appearing in the RGEs of the quark invariants are of the same form as $I_e^{(4)}$ and can be decomposed in the same way into invariants which are in the set. In addition, the RGEs generate two more invariant structures, $I_u' = \mathrm{Re}\,\mathrm{Tr}\left((X_u X_d X_u + \{X_d, X_u^2\})\tilde{Y}_u Y_u^\dagger + X_u^3 \tilde{Y}_d Y_d^\dagger\right)$ and I_d' $(= I_u'(u \leftrightarrow d))$, which can be decomposed into invariants which are already in the set and therefore vanish iff the couplings come from a shift invariant axion. For details on the decomposition and the form of $I_{u,d}'$ in terms of invariants in the set, see App. 6.A.2.

We also want to highlight the form of the RGE of the CP-even invariant $I_{ud}^{(4)}$ which is strongly constrained since $I_{ud}^{(4)}$ is the only CP-conserving invariant in the set. The invariant can only flow into itself and a set of CP-odd invariants multiplied by the Jarlskog invariant $J_4 = \mathrm{Im}\,\mathrm{Tr}\big([X_u, X_d]^3\big)$ where the set of CP-odd invariants is further constrained by the mass dimension of $I_{ud}^{(4)}$. This is exactly what we find in Eq. (6.63) up to the prefactors of the terms, which can only be determined by an explicit computation.

The minimal set in Eq. (6.23), which gives a full rank transfer matrix even for degenerate fermion masses, contains the sum of $I_u^{(3)}$ and $I_d^{(3)}$, which – as shift-breaking invariants themselves – evolve independently under RG flow as can be seen in Eq. (6.63). Therefore, the RG evolution will not only generate $I_u^{(3)} + I_d^{(3)}$, which is contained in the minimal set in Eq. (6.23), but also $I_u^{(3)} - I_d^{(3)}$ and the set only closes under RG flow if the difference can be decomposed in terms of invariants in the minimal set. Following numerical techniques described in Refs. [220, 250, 252], we indeed find a CP-odd relation including all 11 invariants in the redundant set at dimension 12[8] of a similar form as Eq. (6.62) that allows us to decompose the difference of $I_u^{(3)}$ and $I_d^{(3)}$ in terms of the remaining invariants. However, since at dimension 12 there exist many monomials built from the SM flavour invariants the relation is very complicated and we will not present it here.

Thanks to this relation we can always find a minimal set of invariants that is closed under RG flow. This is still true when the relation becomes trivial due to some of the SM Yukawa couplings being degenerate or the CKM having texture zeros, since the number of necessary relations is sufficiently small and we can start with a smaller minimal set for which it is straightforward to compute that it is closed under RG flow.

6.4.2 RG Running Below the Electroweak Scale and EDM Bounds

Now, we will turn to the discussion of the RG running of shift-breaking flavour invariants in the quark sector below the electroweak scale. This will allow us to connect them to experiments which mostly run at scales of a few GeV. We have derived the conditions for shift invariance in the IR in Eq. (6.53), and, using the expressions of Ref. [213] for the RGEs of the dimension-5 Wilson coefficient, it is straightforward to work out the RGEs of the associated set of flavour invariants to the leading order in $1/f$

$$\dot{I}_x^{(n,\mathrm{IR})} = -12(1+n)(q_x^2 e^2 + C_F g_3^2) I_x^{(n,\mathrm{IR})}\,, \tag{6.64}$$

with $x = u, d$, q_x the electric charge and $C_F = \frac{N_c^2-1}{2N_c} = \frac{4}{3}$, with N_c the number of colours. e and g_3 are the electromagnetic and the $SU(3)_C$ coupling constants, respectively. The running is therefore consistent with the fact that, assuming an exact axion shift symmetry at the matching scale, the invariants $I_x^{(n,\mathrm{IR})}$ will continue to vanish at any scale where the EFT expansion is meaningful.

We explained in Section 6.3.3 that the IR conditions for shift symmetry do not correlate the up and down sectors due to the absence of $SU(2)_L$ gauge interactions below the EW scale. Nevertheless, in a top-down approach assuming a matching to a linear phase of the EW symmetry and an approximate axion shift symmetry, it is possible to tune all UV flavour

[8] Where the dimension is defined such that $\dim(X_{u,d}) = 1$ as well as $\dim(\tilde{Y}_{u,d} Y_{u,d}^\dagger) = 1$.

invariants in Eq. (6.21) at the matching scale to very small values, including those which do not belong to the IR set. Including higher order corrections in the EFT below the EW scale, corresponding to the axion-independent part of the EFT, we then find that the RG flow to smaller energies respects the power counting imposed at the matching scale by the shift symmetry, at leading order.

Since we integrate out the top, it is convenient to use a flavour basis, which describes mass eigenstates in the up sector, such as the basis of Eq. (6.5). The matching relations between the couplings in Eqs. (6.1) and (6.2) and those in the IR basis of Eqs. (6.51) and (6.52) then read

$$m_d = \frac{v}{\sqrt{2}}\text{diag}(y_d, y_s, y_b)\ , \quad m_u = \frac{v}{\sqrt{2}}\text{diag}(y_u, y_c)\ , \quad \tilde{m}_d = \frac{v}{\sqrt{2}}V_{\text{CKM}}^\dagger \tilde{Y}_d\ , \quad \tilde{m}_u = \frac{v}{\sqrt{2}}\tilde{Y}_u^{2\times2}\ , \tag{6.65}$$

where v is the Higgs VEV and $M^{2\times2}$ refers to the first two rows and columns of any matrix M. When the shift symmetry is exact in the EFT above the electroweak scale, namely that the relations in Eq. (6.4) hold, the matching conditions in Eq. (6.65) imply that, at the matching scale, all the UV invariants keep on vanishing when one replaces $Y_u, \tilde{Y}_u$ with $Y_u^{\text{IR}}, \tilde{Y}_u^{\text{IR}}$, where

$$Y_u^{\text{IR}} \equiv \begin{pmatrix} Y_u^{2\times2} & 0 \\ 0 & 0 \end{pmatrix}\ , \quad \tilde{Y}_u^{\text{IR}} \equiv \begin{pmatrix} \tilde{Y}_u^{2\times2} & 0 \\ 0 & 0 \end{pmatrix}\ . \tag{6.66}$$

This follows from the fact that, in a basis such as that of Eq. (6.5) where $Y_u = \begin{pmatrix} Y_u^{2\times2} & 0 \\ 0 & y_t \end{pmatrix}$, we can perform the same construction

$$i\left(\tilde{Y}_u^{\text{IR}} Y_u^{\text{IR}\dagger} + h.c.\right) = \left[c_Q, Y_u^{\text{IR}} Y_u^{\text{IR}\dagger}\right]\ , \tag{6.67}$$

as we have done in the UV in Eq. (6.18). As an example, we apply this replacement to the simplest UV invariant which connects the up and down sectors, $I_{ud}^{(1)}$, which yields

$$I_{ud}^{(1,\text{IR})} \equiv \text{Re}\,\text{Tr}\Big(V_{\text{CKM}} m_d m_d^\dagger V_{\text{CKM}}^\dagger \tilde{m}_u m_u^\dagger + V_{\text{CKM}} \tilde{m}_d m_d^\dagger V_{\text{CKM}}^\dagger m_u m_u^\dagger\Big) = 0\ , \tag{6.68}$$

where the sum over the elements of CKM matrix only runs over the first two rows.

In order to study the fate of $I_{ud}^{(1,\text{IR})}$ under RG running, we need to fully express the flavourful couplings in it in terms of IR data. In particular, factor of V_{CKM} appear in the invariant, which does not exist in the renormalisable Lagrangian below the electroweak scale. Instead, we have to map it to non-renormalisable couplings generated when the SM particles are integrated out from the theory. Indeed, integrating out the W boson at tree level from the SM (supplemented by the couplings of Eq. (6.1)), one finds at $\mathcal{O}(1/v^2)$ only one four-quark operator which depends on the CKM matrix.[9]

$$\mathcal{L} \supset -\frac{4}{v^2} V_{\text{CKM},pr} V^*_{\text{CKM},ts} \bar{u}_{L,p}\gamma^\mu d_{L,r} \bar{d}_{L,s}\gamma^\mu u_{L,t} \equiv L^{V1,LL}_{uddu,prst} \mathcal{O}^{V1,LL}_{uddu,prst} \,, \tag{6.69}$$

as well as a semi-leptonic operator containing a single CKM matrix. Using the four-quark operator, where the tensor product of two CKM matrices is less suppressed, we can therefore reexpress our UV invariant $I^{(1,\text{IR})}_{ud}$ as

$$I^{(1,\text{IR})}_{ud} \propto \text{Re}\left(L^{V1,LL}_{uddu,prst} \left[\left(m_d m_d^\dagger\right)_{rs} \left(\tilde{m}_u m_u^\dagger\right)_{tp} + \left(\tilde{m}_d m_d^\dagger\right)_{rs} \left(m_u m_u^\dagger\right)_{tp} \right] \right) \tag{6.70}$$

where every quantity appearing is now a genuine IR coupling. Assuming an axion shift symmetry, tree-level matching imposes $I^{(1,\text{IR})}_{ud} = 0$ at the electroweak scale, and it turns out that it remains zero at lower energies (at least to the one-loop, leading-log and $\mathcal{O}(1/(fv^2))$ order that we checked). Indeed, RG running of the axion couplings at $\mathcal{O}(1/f)$ [213] implies that

$$\begin{aligned} &\mu \frac{d}{d\mu} \left[\left(m_d m_d^\dagger\right)_{rs} \left(\tilde{m}_u m_u^\dagger\right)_{tp} + \left(\tilde{m}_d m_d^\dagger\right)_{rs} \left(m_u m_u^\dagger\right)_{tp} \right] \\ &\quad = -12\left(2C_F g_3^2 + (q_u^2 + q_d^2)e^2\right) \left[\left(m_d m_d^\dagger\right)_{rs} \left(\tilde{m}_u m_u^\dagger\right)_{tp} + \left(\tilde{m}_d m_d^\dagger\right)_{rs} \left(m_u m_u^\dagger\right)_{tp} \right] \,, \end{aligned} \tag{6.71}$$

which keeps the set of invariants closed under the part of the RG flow induced by the axion couplings. The operators generated by integrating out the heavy particles from the SM at tree level are all of the type vector current-vector current [291, 292]. Therefore, we can restrict the RG running of the four-fermion operator parameterising the effects of the CKM matrix at low energies at $\mathcal{O}(1/v^2)$ immensely. Indeed, the vector-vector Wilson coefficients, which we generically denote L_{prst}, do not contribute to the running of coefficients of another kind (such as scalar, tensor or dipole operators). They run into themselves, other L_{prst} and structures such as $\delta_{pt} L_{wrsw}$. Therefore, flavour invariants of the form

$$\text{Re}\left(L_{prst} \left[\left(m_d m_d^\dagger\right)_{rs} \left(\tilde{m}_u m_u^\dagger\right)_{tp} + \left(\tilde{m}_d m_d^\dagger\right)_{rs} \left(m_u m_u^\dagger\right)_{tp} \right] \right) \tag{6.72}$$

run into themselves, identical invariants with other L_{prst} as well as invariants of the form

$$\text{Re}\left(\delta_{pt} L_{wrsw} \left[\left(m_d m_d^\dagger\right)_{rs} \left(\tilde{m}_u m_u^\dagger\right)_{tp} + \left(\tilde{m}_d m_d^\dagger\right)_{rs} \left(m_u m_u^\dagger\right)_{tp} \right] \right) \,. \tag{6.73}$$

This second kind of invariants runs into itself as well as structures where $\delta_{pt} L_{wrsw} \to \delta_{pt}\delta_{rs} L_{wxxw}$ (due to the properties of the CKM matrix), where the last factor can be taken out of the real

[9] After performing spinor and colour Fierz identities, we can identify the operator $\mathcal{O}^{V1,LL}_{uddu,prst}$ and its octet form with the operators $\mathcal{O}^{V1,LL}_{ud,prst}, \mathcal{O}^{V8,LL}_{ud,prst}$ of the LEFT basis of [291], and their Wilson coefficients with $L^{V1,LL}_{ud,prst}, L^{V8,LL}_{ud,prst}$. More precisely, $\mathcal{O}^{V1,LL}_{uddu,prst} = \frac{1}{N_c}\mathcal{O}^{V1,LL}_{ud,ptsr} + 2\mathcal{O}^{V8,LL}_{ud,ptsr}$ and $\mathcal{O}^{V8,LL}_{uddu,prst} = \frac{c_F}{N_c}\mathcal{O}^{V1,LL}_{ud,ptsr} - \frac{1}{N_c}\mathcal{O}^{V8,LL}_{ud,ptsr}$, where the octet operator $\mathcal{O}^{V8,LL}_{uddu,prst}$ is not generated by integrating out the W at tree level but will appear in the RG running of $\mathcal{O}^{V1,LL}_{uddu}$.

part due to the hermitian properties of the vector-vector operators. Finally, invariants of the form L_{wxxw} only run into themselves. Therefore, taking into account the running and the boundary conditions of the 4-fermion operators at the matching scale, these IR flavour-invariant structures form a RG-closed space.

In particular, if they all vanish at the matching scale, they all remain equal to zero at lower energies at the order that we checked. Similarly, if they are suppressed by a small parameter at the matching scale, they remain suppressed by that parameter at lower energies. In addition, as anticipated above, the fact that they vanish (or are suppressed) follows from an exact (or approximate) axion shift symmetry. This symmetry is of course not broken by integrating out the heavy particles from the theory but instead the correlations introduced by the $SU(2)$ gauge symmetry get pushed to higher mass dimensions in the low-energy EFT. Indeed, at the matching scale, all L_{prst} have a flavour structure given by combinations of $V_{\text{CKM},pr}V^*_{\text{CKM},ts}$, $V_{\text{CKM},pr}\delta_{st}$ and $\delta_{pt}\delta_{rs}$. Hence, at the matching scale, the above IR invariants are proportional to combinations of $I^{(1,\text{IR})}_{ud}$ and $\text{Tr}\left(m_d m_d^\dagger\right)I^{(1,\text{IR})}_u + \text{Tr}\left(m_u m_u^\dagger\right)I^{(1,\text{IR})}_d$ and all vanish for an exact shift symmetry. Therefore, assuming an exact (or approximate) axion shift symmetry in the UV makes all the above IR invariants, in particular $I^{(1,\text{IR})}_{ud}$, vanishing (or small) at the matching scale as well as at any lower energy.

The stability of the constraints under RG flow allows us to use them at low energies, and to identify the impact of an approximate shift symmetry on bounds on the couplings of Eq. (6.52) derived from observables. The consequences are twofold: *(i)* the fundamental parameter space constrained by the bounds is reduced, and *(ii)* sum rules between different observables are predicted. We illustrate these two aspects by reanalysing the bounds derived in [282], where the authors study electric dipole moments and allow for shift-breaking couplings in the generic basis of Eq. (6.52).

Bounds on the ALP couplings can be set using experimental bounds on the spin precession frequency ω_{ThO} of the polar molecule ThO, the neutron EDM d_n and the EDM d_{Hg} of the diamagnetic atom ^{199}Hg

$$\begin{aligned} \omega_{\text{ThO}} &< 1.3\,\text{mrad/s}\ (90\%\ \text{C.L.})\ , \\ d_n &< 1.8 \times 10^{-26}\, e\,\text{cm}\ (90\%\ \text{C.L.})\ , \\ d_{\text{Hg}} &< 6 \times 10^{-30}\, e\,\text{cm}\ (90\%\ \text{C.L.})\ . \end{aligned} \tag{6.74}$$

The expressions of these quantities are given in Ref. [282] in terms of the couplings[10] $\tilde{m}$ of Eq. (6.52), as well as CP-even and odd couplings of the axion to gluons and photons, under the assumption that the axion mass is of order a few GeV's so that the axion can be integrated out while QCD can still be treated perturbatively.

Let us study the fate of these bounds when the axion shift symmetry is approximate. More precisely, we assume that any shift-breaking coupling is generated by particles at the PQ scale f and that a single spurion ϵ breaks the PQ symmetry. For instance, this suggests writing $m_a^2 = \mathcal{O}(\epsilon f^2)$ for the axion mass, or $\mathcal{I} = \mathcal{O}(\epsilon)$ for any of our shift-breaking invariants $\mathcal{I}$. Working in the basis where masses are diagonal and real, the ϵ-scaling of the IR invariants

[10] Matching to our notations, y_S and y_P of Ref. [282] are respectively the hermitian and anti-hermitian parts of $\tilde{m}$, for each kind of fermion.

imply for instance that

$$(\tilde{m}_x + \tilde{m}_x^\dagger)_{ii} = \mathcal{O}(\epsilon) \ , \tag{6.75}$$

for any fermion species x, reducing the number of coefficients contributing at the considered accuracy in ϵ. Additionally, CP-odd axion-gluon or axion-photon couplings break the shift symmetry, and are therefore $\mathcal{O}(\epsilon)$. The EDM of mercury is a function of the EDM of the neutron EDM, as well as effective electron-neutron four-fermion operators [282]. All of these can in turn be mapped to effective operators of electrons coupled to quarks and gluons. After integrating out the axion at 1-loop, one can identify the shift invariants in the matching contributions of these effective operators appearing in the expressions of the EDMs. Hence, working at order $\mathcal{O}(\epsilon^0/f^2)$ (we also assume $v^2/f^2 \lesssim \epsilon$ and count $\log\epsilon = \mathcal{O}(1)$), one obtains from Ref. [282] that

$$d_{\mathrm{Hg}} \simeq 4\times 10^{-4} d_n \,, \tag{6.76}$$

which is an example of a sum rule between observables following from the axion shift-symmetry.

The only remaining combinations induced at 1-loop by a shift-symmetric axion above the QCD scale, which cannot immediately be identified with our invariants, are the axion-induced EDMs d_i and chromo-EDMs d_i^C of fundamental fermions ψ_i, which read [282]

$$\frac{d_i}{e} = Q_i d_i^C \ , \quad d_i^C \simeq \frac{2}{16\pi^2 f^2} \mathrm{Im}\left(\tilde{m} m^{-1} \tilde{m}\right)_{ii} \ , \tag{6.77}$$

with Q_i the electric charge. The same combination of quark (chromo-)EDMs enters d_n and d_{Hg}, hence the related bounds yield constraints on the same combination of fundamental parameters $\tilde{m}$, which turn out to be of very similar magnitude.

The other bounds of Eq. (6.74) yield more independent bounds on the EDMs of fundamental fermions. For instance, the bound on ω_{ThO} turns into a bound on the electron EDM

$$d_e \lesssim 10^{-29}\, e\,\mathrm{cm} \ . \tag{6.78}$$

It is natural to expect that the contribution of the tau lepton dominates,[11] and one finds

$$\left|\frac{\mathrm{Im}\left(\tilde{m}_{e\tau}\tilde{m}_{\tau e}\right)}{m_\tau^2}\right| = \left|\mathrm{Im}\left(c_{L,13} c_{e,31}\right)\right| \lesssim 1.4 \left(\frac{f}{10^8 \mathrm{GeV}}\right)^2 \ , \tag{6.79}$$

where we expressed the bound in terms of the CP-violating couplings of Eq. (6.3), which can be used at $\mathcal{O}(\epsilon^0)$ we are interested in, while at higher orders in ϵ also potential shift-breaking terms can contribute which are not captured by the $C_{Q,u,d,L,e}$. Similarly, the bounds on d_n and d_{Hg} reduce to bounds of similar magnitude on the same combination of quark EDMs, ,

$$\left(\frac{2}{3}0.784(28) - 0.55(28)\right) d_u^C - \left(1.10(55) - \frac{1}{3}0.294(11)\right) d_d^C \lesssim 10^{-26}\mathrm{cm} \ . \tag{6.80}$$

[11] This follows from the generic form of axion couplings at $\mathcal{O}(\epsilon^0)$ given in Eq. (6.4), and it can be checked in the Froggatt–Nielsen or 2HDM examples above that, generically, $\tilde{m}_{e,13} \sim \mathcal{O}(1) m_\tau$.

Although the combined coefficient of the up-contribution suffers from large uncertainties, it is numerically suppressed (~ 0.03), so that its top-mediated component does not dominate over the bottom contribution in the respective expressions of $d^C_{u,d}$, due to the numerical value of m_b/m_t which is ~ 0.02. Therefore, we expect the generic bound to combine the top and bottom contribution. For illustration purposes, let us assume that the bottom contribution dominates, which at $\mathcal{O}(\epsilon^0)$ leads to

$$\left|\frac{\mathrm{Im}\,(\tilde{m}_{db}\tilde{m}_{bd})}{m_b^2}\right| = \left|\mathrm{Im}\left(c_{Q,13}c_{d,31}\right)\right| \lesssim 1.1 \times 10 \left(\frac{f}{10^7\mathrm{GeV}}\right)^2 \,. \tag{6.81}$$

In addition, the ϵ-scaling of $I^{(1,\mathrm{IR})}_{ud}$ of Eq. (6.70) further correlates the entries of $\tilde{m}$ which contribute to the different EDMs. However, this does not generate more sum rules between observables at $\mathcal{O}(\epsilon^0/f^2)$. In the meantime, the analysis presented here has been performed in more details in Ref. [286], making use of the invariants presented in this chapter.

6.4.3 ALP-SMEFT Interference and Sum Rules

If the presence of an axion is detected, it will be crucial to learn more about its couplings, in particular to SM fermions. However, those may be difficult to probe, and indirect probes will play an important role in constraining them. The axion-induced RG running of couplings between SM particles is a good example, as it will generically deviate from that of a situation without any axion.

Assuming no further light degree of freedom, the couplings of SM particles can be captured by the SMEFT. The presence of an axion induces an RG evolution of the dimension-6 pure SMEFT couplings driven by the dimension-5 axion couplings [293], which deviates from that in the pure SMEFT [94–97]. In this section, we will discuss how to extract information about properties of the axion from these deviations. Our invariants will allow us to immediately identify implications of the axion shift symmetry, in the form of flavour-invariant sum rules on the RG evolution of the SMEFT Wilson coefficients.

We define the terms sourcing the deviations from the SMEFT RGEs induced by the ALP EFT as follows [293],

$$\mu\frac{dC_i^{\mathrm{SMEFT}}}{d\mu} - \gamma_{ji}^{\mathrm{SMEFT}}C_j^{\mathrm{SMEFT}} \equiv \frac{S_i}{(4\pi f)^2} \,. \tag{6.82}$$

In particular, those source terms which only contain one flavourful axion coupling or which contain a tensor product of two axion couplings will be useful, as they will allow us to immediately connect them to our invariants. For instance, we can use the following source terms [293]

$$\begin{aligned} S_{uG} &= -4ig_s\tilde{Y}_u C_{GG}, & S_{dG} &= -4ig_s\tilde{Y}_d C_{GG}, \\ S_{uW} &= -ig_2\tilde{Y}_u C_{WW}, & S_{dW} &= -ig_2\tilde{Y}_d C_{WW}, \\ S_{uB} &= -2ig_1(y_Q+y_u)\tilde{Y}_u C_{BB}, & S_{dB} &= -2ig_1(y_Q+y_d)\tilde{Y}_d C_{BB}, \end{aligned} \tag{6.83}$$

to write

$$\begin{aligned}\mathrm{Im}\,\mathrm{Tr}\left(X_x^{0,1,2}S_{xG}Y_x^\dagger\right) &= -4g_sC_{GG}I_x^{(1,2,3)}\\ \mathrm{Im}\,\mathrm{Tr}\left(X_x^{0,1,2}S_{xW}Y_x^\dagger\right) &= -g_2C_{WW}I_x^{(1,2,3)}\\ \mathrm{Im}\,\mathrm{Tr}\left(X_x^{0,1,2}S_{xB}Y_x^\dagger\right) &= -g_1(y_Q+y_x)C_{BB}I_x^{(1,2,3)}\end{aligned} \tag{6.84}$$

with $x = u, d$ and all Wilson coefficients which have not been defined previously can be found in Tab. 6.3. Furthermore, we can use the source terms in Eq. (6.83) which only depend on the type of the fermion through the dimension-5 Yukawa to write down relations for the mixed invariants. For the gluon source terms we find e.g.

$$\mathrm{Im}\,\mathrm{Tr}\left(X_dX_uX_dS_{uG}Y_u^\dagger + X_uX_dX_uS_{dG}Y_d^\dagger\right) = -4g_sC_{GG}I_{ud}^{(3)} \tag{6.85}$$

and similar expressions for the W-boson source terms. Furthermore, we can find relations in terms of our invariants where the ALP-fermion couplings appear in tensor products. This is the case for some 4-fermion operators. E.g. combining the source terms [293]

$$\left(S_{qx}^{(1)}\right)_{prst} = \frac{1}{N_c}\left(\tilde{Y}_x\right)_{pt}\left(\tilde{Y}_x^\dagger\right)_{sr} + \frac{16}{3}g_1^2y_Qy_xC_{BB}^2\delta_{pr}\delta_{st} \tag{6.86}$$

with $x = u, d$ we can find the following relation

$$\begin{aligned}\mathrm{Re}\Bigg(\left(S_{qu}^{(1)}\right)_{prst}\left(Y_u^\dagger\right)_{tp}\left(Y_u\right)_{rs} - \frac{y_u\,\mathrm{Tr}(X_u)}{y_d\,\mathrm{Tr}(X_d)}\left(S_{qd}^{(1)}\right)_{prst}\left(Y_d^\dagger\right)_{tp}\left(Y_d\right)_{rs}\Bigg)&\\ = \frac{1}{N_c}\left(\left(I_u^{(1)}\right)^2 - \frac{y_u\,\mathrm{Tr}(X_u)}{y_d\,\mathrm{Tr}(X_d)}\left(I_d^{(1)}\right)^2\right)&,\end{aligned} \tag{6.87}$$

where the y_i are the hypercharges of the SM fermions. Finally, with the source term [293]

$$\left(S_{ledq}\right)_{prst} = -2\left(\tilde{Y}_e\right)_{pr}\left(\tilde{Y}_d^\dagger\right)_{st} \tag{6.88}$$

we can write

$$\mathrm{Re}\left(\left(S_{ledq}\right)_{prst}\left(Y_e^\dagger\right)_{rp}\left(Y_d\right)_{ts}\right) = -2I_e^{(1)}I_d^{(1)}. \tag{6.89}$$

The sum rules of this type give zeroes in the RG evolution of the SMEFT Wilson coefficients if the ALP is shift symmetric, i.e. the RG evolution of the precise combination of SMEFT Wilson coefficients appearing in the sum rule is completely determined by SMEFT Wilson coefficients. Said differently, observing RGEs compatible with the SMEFT for the combinations of Wilson coefficients entering the above sum rules suggests that the axion shift symmetry is weakly broken. The uncertainty in the measurements of the SMEFT coefficients quantifies which room there remains for non-vanishing invariants, i.e. for shift-symmetry breaking.

SMEFT	ALP EFT
$\mathcal{O}_{q_R G} = \bar{Q}\sigma^{\mu\nu}T^a q_R H_{(q_R)} G^a_{\mu\nu}$	$\mathcal{O}_{GG} = \frac{a}{f} G^a_{\mu\nu}\tilde{G}^{\mu\nu,a}$
$\mathcal{O}_{q_R W} = \bar{Q}\sigma^{\mu\nu}\sigma^I q_R H_{(q_R)} W^I_{\mu\nu}$	$\mathcal{O}_{WW} = \frac{a}{f} W^I_{\mu\nu}\tilde{W}^{\mu\nu,I}$
$\mathcal{O}_{q_R B} = \bar{Q}\sigma^{\mu\nu} u H_{(q_R)} B_{\mu\nu}$	$\mathcal{O}_{BB} = \frac{a}{f} B_{\mu\nu}\tilde{B}^{\mu\nu}$
$\mathcal{O}^{(1)}_{qq_R} = \left(\bar{Q}\gamma_\mu Q\right)\left(\bar{q_R}\gamma^\mu q_R\right)$	
$\mathcal{O}_{ledq} = \left(\bar{L}e\right)\left(\bar{d}Q\right)$	

Table 6.3: Additional EFT operators of the SMEFT and ALP EFT as defined in Ref. [293] that enter in the sum rules and have not been defined previously. q_R stands for u, d and $H_{(u)} \equiv \tilde{H}, H_{(d)} \equiv H$.

6.5 Couplings to Gluons and Non-Perturbative Shift Invariance

Previously, we have focused on the breaking of shift-invariance which arises at the perturbative level. This is for instance relevant for interactions which induce axion potentials at the tree or loop levels, as is often discussed in the axion quality problem or relaxion literature. We have, however, neglected axion couplings to gauge bosons of the SM gauge group $SU(3)_C \times SU(2)_W \times U(1)_Y$, and in particular to gluons. The latter do not break the shift symmetry at the perturbative level, but they do so *non-perturbatively*, as we will explore in the context of small instantons in Chap. 8 of this thesis. Furthermore, the coefficient of these couplings change upon the transformation of the two bases discussed throughout this chapter. Hence, a vanishing coupling in one basis might become non-zero in the other basis. In this section, we will work out conditions for the axion couplings to remain shift-symmetric when gluons are taken into account.

To this end, we add the following term to the Lagrangian of Eq. (6.1)

$$-\frac{C_g g_3^2}{16\pi^2}\frac{a}{f}\,\mathrm{Tr}\big(G_{\mu\nu}\tilde{G}^{\mu\nu}\big) \,, \tag{6.90}$$

and to that of (6.3) the same term with $C_g \to C_g^{(s)}$. We use explicitly different notations for clarity, since both couplings will appear in the same relations when we match between the two operator bases. The overall normalisation is chosen consistently with naive dimensional analysis, also keeping in mind the origin of $C_g, C_g^{(s)}$ in UV theories with heavy anomalous fermions, which are such that $C_g, C_g^{(s)} = \mathcal{O}(1)$.

The gluon coupling breaks the shift symmetry *non-perturbatively*, unless at least one quark is massless. In that case, a shift of the axion field $a \to 2\pi\alpha_{\mathrm{PQ}} f$ is equivalent to a shift of $\theta_{\mathrm{QCD}} \to 2\pi\alpha_{\mathrm{PQ}}$, which can be absorbed with an appropriate chiral transformation of the massless quark. Therefore, we assume here that all quarks are massive, so that there are no chiral symmetries of the spectrum, and θ_{QCD} is physical. I.e. the theory differentiates between different values of the axion VEV $\langle a\rangle$ and the shift symmetry is broken, generating an axion potential.

We now follow the same logic as in the perturbative case: we look for quantities which must vanish for the shift invariance to hold non-perturbatively, which are therefore order parameters for the non-perturbative breaking.

6.5.1 Non-Perturbative Order Parameter

Let us first assume, that the axion shift symmetry is exact at the perturbative level. Then, the couplings of the axion to fermions comes in the basis of Eq. (6.3), where all fermion couplings are invariant under a shift of a. At the non-perturbative level, $C_g^{(s)} = 0$ is required to cancel the gluon-induced shift-breaking contributions to the axion potential.

However, as in previous sections, we want to identify order parameters in the most general operator basis, where they could be non-zero in realistic models. This means that we want to derive the equivalent of the condition $C_g^{(s)} = 0$ in terms of the couplings of Eq. (6.1). For that, we need to account for anomalies when we change the operators basis from Eq. (6.3) to Eq. (6.1) with the following field redefinition

$$\psi' \equiv e^{-i\frac{a}{f}c_\psi}\psi \ , \tag{6.91}$$

for each chiral fermion field ψ of the SM. This transformation is anomalous and generates the following matching relation between the coupling to gluons,

$$C_g = C_g^{(s)} + \mathrm{Tr}(2C_Q - C_u - C_d) \ . \tag{6.92}$$

When the gluon couplings do not break the PQ symmetry, $C_g^{(s)} = 0$ and one finds[12]

$$C_g = \mathrm{Tr}(2C_Q - C_u - C_d) \ . \tag{6.93}$$

Once more assuming that all Yukawa couplings are non-zero, we can use the matching conditions of Eq. (6.4) to substitute the coefficients C_i for the $\tilde{Y}_i$

$$C_g - i\,\mathrm{Tr}\left(Y_u^{-1}\tilde{Y}_u + Y_d^{-1}\tilde{Y}_d\right) = 0 \ . \tag{6.94}$$

Note that our assumption of massive quarks make the Yukawa matrices invertible and the expression meaningful. This expression yields an extra condition for a perturbative shift symmetry to remain valid even non-perturbatively in g_3, in the basis of Eq. (6.1). The right-hand side of the above expression is constrained to be imaginary due to our conditions for perturbative shift-invariance of Eq. (6.21), so we find that the new condition is CP-even and reads $I_g = 0$ for

$$I_g \equiv C_g + \mathrm{Im}\,\mathrm{Tr}\left(Y_u^{-1}\tilde{Y}_u + Y_d^{-1}\tilde{Y}_d\right) \ . \tag{6.95}$$

When all the perturbative invariants of Eqs. (6.21)-(6.22) vanish, i.e. when there exists an exact PQ symmetry at the perturbative level, I_g captures the mixed anomaly polynomial of that symmetry with $SU(3)_C$. This can easily be seen in the axiflavon/flaxion model of

[12] For obvious reasons, this relation looks similar to those used to compute perturbative corrections to the θ term in various EFTs [288, 294].

Eq. (6.26), where

$$I_g = \sum_i (2q_{Q_i} - q_{u_i} - q_{d_i}) \ . \tag{6.96}$$

The invariant I_g, which features couplings from the up and down sectors, highlights a new kind of collective breaking at the non-perturbative level, which is consistent with the fact that mixed PQ anomalies can be cancelled by balancing non-vanishing contributions in different quark sectors.

In addition, the derivation never referred to the invariants which correlate the up and down sectors in Eq. (6.21) and are absent in Eq. (6.53), therefore it is valid below the electroweak scale, up to the replacements $Y, \tilde{Y} \to m, \tilde{m}$ to match the notations of section 6.3.3.

6.5.2 RG running

By, once more, using the RGEs of the Standard Model and axion Yukawa couplings above the electroweak scale [212, 213], we can show that all contributions to the running of this invariant cancel at the one-loop level

$$\mu \frac{dI_g}{d\mu} = 0 \ . \tag{6.97}$$

Let us stress that we chose a scaling in Eq. (6.90) similar to that of [212], where C_g already comes with a one-loop factor $g_3^2/(16\pi^2)$. This allowed us to account for the anomalous shift without loop-factor hierarchies in Eq. (6.93). However, when working out the RGEs as in Ref. [213], we also need to account for anomalies and their contribution to the running of C_g. One can show, that with the other normalisation, the invariant has a non-zero RGE, which is only proportional to the invariant itself. This is shown in detail in Ref. [1].

Appendices to Chapter 6

6.A Useful Matrix Relations

6.A.1 Commutator Relations Used in Section 6.2.3

The simplest commutator identity one can write down using three matrices A, B, C is

$$[A, BC] = [A, B]\,C + B\,[A, C] \ . \tag{6.98}$$

Using Eq. (6.18) and the fact that the trace of a commutator vanishes, we obtain

$$-i\,\mathrm{Tr}\left(X_d\left[c_Q, X_u\right] + X_u\left[c_Q, X_d\right]\right) = \mathrm{Tr}\left(X_d\left(\tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger\right) + (u \leftrightarrow d)\right) = 0 \ . \tag{6.99}$$

It is straightforward to generalise the identity in Eq. (6.98) to four and five matrices and obtain identities at higher order in $X_{u,d}$. For any four matrices A, B, C, D we have

$$[A, BCD] = [A, B]\,CD + B\,[A, C]\,D + BC\,[A, D] \,. \tag{6.100}$$

Identifying $A = c_Q, B = X_u, C = D = X_d$ and tracing over both sides gives

$$\mathrm{Tr}\left(X_d^2\left(\tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger\right) + \{X_d, X_u\}\left(\tilde{Y}_d Y_d^\dagger + Y_d \tilde{Y}_d^\dagger\right)\right) = 0 \ . \tag{6.101}$$

This expression is not symmetric under $u \leftrightarrow d$, allowing us to find another independent condition by exchanging $u \leftrightarrow d$,

$$\mathrm{Tr}\left(X_u^2\left(\tilde{Y}_d Y_d^\dagger + Y_d \tilde{Y}_d^\dagger\right) + \{X_d, X_u\}\left(\tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger\right)\right) = 0 \ . \tag{6.102}$$

The following identity involving five generic matrices A, B, C, D, E,

$$[A, BCDE] = [A, B]\,CDE + B\,[A, C]\,DE + BC\,[A, D]\,E + BCD\,[A, E] \ , \tag{6.103}$$

allows us to find a fourth condition

$$\mathrm{Tr}\left(X_d X_u X_d\left(\tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger\right) + X_u X_d X_u\left(\tilde{Y}_d Y_d^\dagger + Y_d \tilde{Y}_d^\dagger\right)\right) \ , \tag{6.104}$$

and the final condition which we consider derives from applying the Jacobi identity on Eq. (6.18),

$$\begin{aligned} \left[X_u, \tilde{Y}_d Y_d^\dagger + Y_d \tilde{Y}_d^\dagger\right] - \left[X_d, \tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger\right] &= -i\left(\left[X_u, \left[c_Q, X_d\right]\right] + \left[X_d, \left[X_u, c_Q\right]\right]\right) \\ &= i\left[c_Q, \left[X_d, X_u\right]\right] \ , \end{aligned} \tag{6.105}$$

so that Eq. (6.19) yields

$$\mathrm{Tr}\left(\left[X_u, X_d\right]^n \left(\left[X_u, \tilde{Y}_d Y_d^\dagger + Y_d \tilde{Y}_d^\dagger\right] - \left[X_d, \tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger\right]\right)\right) = 0 \ . \tag{6.106}$$

We only make use of the condition where $n = 2$.

The above expressions can be made more compact by noticing that, for any two hermitian matrices H_u, H_d, we can write

$$\begin{aligned} &\mathrm{Tr}\left(H_u(\tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger) + H_d(\tilde{Y}_d Y_d^\dagger + Y_d \tilde{Y}_d^\dagger)\right) = \mathrm{Tr}\left(H_u \tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger H_u^\dagger + (u \leftrightarrow d)\right) \\ &= \mathrm{Tr}\left(H_u \tilde{Y}_u Y_u^\dagger\right) + \mathrm{Tr}\left(H_u \tilde{Y}_u Y_u^\dagger\right)^* + (u \leftrightarrow d) = 2\mathrm{Re}\,\mathrm{Tr}\left(H_u \tilde{Y}_u Y_u^\dagger\right) + (u \leftrightarrow d) \ . \end{aligned} \tag{6.107}$$

For two anti-hermitian matrices A_u, A_d, one similarly finds

$$\mathrm{Tr}\left(A_u(\tilde{Y}_u Y_u^\dagger + Y_u \tilde{Y}_u^\dagger) + A_d(\tilde{Y}_d Y_d^\dagger + Y_d \tilde{Y}_d^\dagger)\right) = 2i\mathrm{Im}\,\mathrm{Tr}\left(A_u \tilde{Y}_u Y_u^\dagger\right) + (u \leftrightarrow d) \ . \tag{6.108}$$

6.A.2 Details on Decomposition of Invariants Generated by RG Flow

In the RGEs of the invariants we find invariants which naively are not in the minimal set. However they can be decomposed into invariants in the set which we will show here in detail. Apart from $I_u^{(4)}, I_d^{(4)}$ which can be decomposed in an analogous way as $I_e^{(4)}$, the RG evolution also generates, $I_u' = \mathrm{Re}\,\mathrm{Tr}\left(\left(X_u X_d X_u + \{X_d, X_u^2\}\right)\tilde{Y}_u Y_u^\dagger + X_u^3 \tilde{Y}_d Y_d^\dagger\right)$ and I_d' $(= I_u'(u \leftrightarrow d))$, which are redundant as we will see now. As before we can construct the invariants generated by the RG flow of the original set by using again the commutator relation in Eq. (6.103) with $A = c_Q, B = C = E = X_u, D = X_d$ for I_u' and $A = c_Q, B = C = E = X_d, D = X_u$ for I_d'. To see that the invariants are not independent of the invariants in Eq. (6.21) we have to employ the Cayley-Hamilton theorem. Multiplying Eq. (6.61) by A, taking the trace, replacing $A \to A + B + C$ and only keeping terms of order A^2BC we find the following relation [218]

$$\begin{aligned} 0 = &\mathrm{Tr}(A)^2\,\mathrm{Tr}(B)\,\mathrm{Tr}(C) - \mathrm{Tr}(BC)\,\mathrm{Tr}(A)^2 - 2\,\mathrm{Tr}(AB)\,\mathrm{Tr}(A)\,\mathrm{Tr}(C) - 2\,\mathrm{Tr}(AC)\,\mathrm{Tr}(A)\,\mathrm{Tr}(B) \\ &+ 2\,\mathrm{Tr}(ABC)\,\mathrm{Tr}(A) + 2\,\mathrm{Tr}(ACB)\,\mathrm{Tr}(A) - \mathrm{Tr}\left(A^2\right)\mathrm{Tr}(B)\,\mathrm{Tr}(C) + 2\,\mathrm{Tr}(AB)\,\mathrm{Tr}(AC) \\ &+ \mathrm{Tr}\left(A^2\right)\mathrm{Tr}(BC) + 2\,\mathrm{Tr}(C)\,\mathrm{Tr}\left(A^2B\right) + 2\,\mathrm{Tr}(B)\,\mathrm{Tr}\left(A^2C\right) - 2\,\mathrm{Tr}\left(A^2BC\right) - 2\,\mathrm{Tr}\left(A^2CB\right) \\ &- 2\,\mathrm{Tr}(ABAC). \end{aligned} \tag{6.109}$$

By identifying $A = X_u, B = X_d, C = \tilde{Y}_u Y_u^\dagger$ the last three single trace terms in Eq. (6.109) are the same as the terms containing $\tilde{Y}_u Y_u^\dagger$ in I_u'. Using this decomposition and Eq. (6.61) for the

X_u^3 term in I_u' we find

$$\begin{aligned}
I_u' =& \frac{1}{2} I_u^{(1)} \left(\mathrm{Tr}(X_u)^2 \,\mathrm{Tr}(X_d) - \mathrm{Tr}\!\left(X_u^2\right) \mathrm{Tr}(X_d) + 2\,\mathrm{Tr}\!\left(X_u^2 X_d\right) - 2\,\mathrm{Tr}(X_u)\,\mathrm{Tr}(X_u X_d)\right) \\
&+ 2 I_u^{(2)} \left(\mathrm{Tr}(X_u X_d) - \mathrm{Tr}(X_u)\,\mathrm{Tr}(X_d)\right) + 2\,\mathrm{Tr}(X_d) I_u^{(3)} + \frac{1}{2}\left(\mathrm{Tr}\!\left(X_u^2\right) - \mathrm{Tr}(X_u)^2\right) I_{ud}^{(1)} \\
&+ \mathrm{Tr}(X_u) I_{ud,u}^{(2)} + \frac{1}{6}\left(\mathrm{Tr}(X_u)^3 - 3\,\mathrm{Tr}\!\left(X_u^2\right) \mathrm{Tr}(X_u) + 2\,\mathrm{Tr}\!\left(X_u^3\right)\right) I_d^{(1)} \ ,
\end{aligned} \tag{6.110}$$

and a similar decomposition for I_d'.

7

The Hilbert Series of ALP EFTs

7.1 Introduction

In Chap. 6, we have made a first step in understanding PQ-breaking effects in the EFT of ALPs by formulating the breaking effects in flavour-invariant order parameters. In this chapter, we want to carry on this analysis by explicitly studying how these effects are encoded in operators at higher mass dimensions. One main realisation of the work in the previous chapter was that the same operators coupling the ALP to fermions describe both shift-breaking and shift-preserving interactions. This made it difficult to impossible to give the interactions their appropriate power counting which can be very different as the scales of spontaneous and explicit PQ-breaking are usually well-separated. Here, we want to study if this mixing between the shift-breaking and shift-preserving sector continues at higher mass dimensions. To this end, we will build an operator basis for a pseudoscalar with and without a shift symmetry coupled to the SM degrees of freedom.

The operator basis we derive could prove useful for phenomenological as well as theoretical studies. Most analyses study the leading dimension-5 interactions of the ALPs, while some also consider effects from higher dimensional operators at dimension 6 [188, 196, 295–297] and dimension 7 [196, 296, 298]. In particular, the analyses at dimension 7 use an incomplete basis, which may lead to the omission of contributions from other operators that could alter the results of these studies. On the more theoretical side, the operators at dimension 8 are of interest for the discussion of positivity in the context of the ALP EFT. Furthermore, it could be of value for matching calculations [299] to have a complete set of operators beyond the leading interactions. An important probe for new physics are low-energy experiments looking for small corrections in high-precision experiments and exotic decays of mesons involving ALPs (see e.g. Refs. [178, 182, 185, 189, 212]). In order to have a complete effective description of such effects below the electroweak (EW) scale, we will also derive an operator basis for the so called low-energy effective field theory (LEFT) extended with an ALP.

To simplify the procedure of building an operator basis, we will use the Hilbert series techniques introduced in Sec. 2.5.2 to count the number of independent Lorentz- and gauge-invariant operators made from the SM fields below and above the EW scale extended with an ALP with all IBP and EOM redundancies removed. To further investigate the effects of CP violation in the EFTs, we will employ the implementation of CP in the Hilbert series language as was introduced in Sec. 2.5.2, allowing us to perform the counting of CP-even, CP-odd and CP-violating couplings. Since their introduction, these tools have proven helpful in many analyses of different EFTs [64, 85, 105, 215, 225–228, 300–305] to build operator bases and to study different aspects of these EFTs like their behaviour under CP.

We will demonstrate how the Hilbert series can provide a clear and concise understanding of the separation of the shift-symmetric and shift-breaking sectors in the ALP EFTs. We highlight that these two sectors can be distinctly categorised above mass dimension 5, without any observed mixing between them. We will furthermore show that, making a change of basis that is often considered in the literature and convenient to work in in the presence of shift-breaking effects, one has to consider more seemingly shift-breaking operators with completely constrained Wilson coefficients.

7.2 Hilbert Series Techniques for ALP EFTs

We have already introduced most of the necessary tools and jargon in Sec. 2.5.2. As we want to study EFTs of ALPs, in a next step we have to implement the shift symmetry of the ALP in terms of the conformal characters introduced previously.

7.2.1 Implementing the ALP Shift Symmetry

The Hilbert series for theories with shift-symmetric scalars was first discussed in Ref. [64], where a general treatment was introduced within the framework of non-linear realisations of symmetries. This approach has been applied to construct operator bases, such as the operator basis for the shift-symmetric scalar coupled to gravity [301] and for the $O(N)$ non-linear sigma model [228]. Because the axion arises as the Goldstone boson of the spontaneously broken $U(1)_{\text{PQ}}$, we can use the Hilbert series machinery for non-linearly realised symmetries based on the CCWZ construction [173, 174] developed in Ref. [64] to impose its properties in the Hilbert series. It is common to parameterise the Goldstone degrees of freedom $\pi^i(x)$ of a spontaneously broken symmetry $G \to H \subset G$, using the following matrix field

$$\xi(x) = e^{\frac{i\pi^i(x)X^i}{f_\pi}}, \tag{7.1}$$

where X^i are the broken generators living in the coset space G/H and f_π is the pion decay constant. To construct the EFT of the pions of the pions of the spontaneously broken symmetry, one further defines the Cartan form

$$w_\mu \equiv \xi^{-1}\partial_\mu \xi = u^i_\mu X^i + v^a_\mu T^a \equiv u_\mu + v_\mu \tag{7.2}$$

decomposing the degrees of freedom along the broken generators X^i and the unbroken generators T^a. As the ALP is the Goldstone boson of the simple symmetry breaking pattern $U(1)_{\text{PQ}} \to \emptyset$, the discussion reduces drastically. There exists only one broken generator and we can simply write

$$\xi = e^{i\frac{a}{f}}, \qquad w_\mu = u_\mu = i\frac{\partial_\mu a}{f}. \tag{7.3}$$

In the following, instead of working with the Cartan form u_μ, we will work with the simplified expression $u_\mu \sim \partial_\mu a$ for the ALP. In order to implement this explicitly shift-symmetric derivative coupling of the ALP, the scalar itself has to be removed from the list of building blocks for the Hilbert series of the EFT, which is achieved by removing the first entry from the single particle module of the scalar in Eq. (2.104). This yields

$$R_{\partial a} = \begin{pmatrix} \partial_{\mu_1} a \\ \partial_{\{\mu_1}\partial_{\mu_2\}} a \\ \partial_{\{\mu_1}\partial_{\mu_2}\partial_{\mu_3\}} a \\ \vdots \end{pmatrix}. \tag{7.4}$$

The first entry of the single particle module in Eq. (2.104) can be removed with the help of conformal characters by applying another shortening condition on top of the previous one in Eq. (2.110) that eliminates the EOM redundancy.[1] By summing over the characters of the remaining elements (note that the first sum starts at $n = 1$ now) of the scalar single particle module, we obtain the character of a shift-symmetric singlet scalar [64]

$$\begin{aligned} \chi_{\partial a}(\mathcal{D}, x) &= \sum_{n=1}^{\infty} \mathcal{D}^{n+d_a} \chi_{\mathrm{Sym}^n(\frac{1}{2},\frac{1}{2})}(x) - \sum_{n=2}^{\infty} \mathcal{D}^{n+d_a} \chi_{\mathrm{Sym}^{n-2}(\frac{1}{2},\frac{1}{2})}(x) \\ &= \mathcal{D}^{d_a}\left(-1 + \sum_{n=0}^{\infty} \mathcal{D}^n \chi_{\mathrm{Sym}^n(\frac{1}{2},\frac{1}{2})}(x) - \sum_{n=2}^{\infty} \mathcal{D}^n \chi_{\mathrm{Sym}^{n-2}(\frac{1}{2},\frac{1}{2})}(x)\right) \\ &= \mathcal{D}\left(\left(1-\mathcal{D}^2\right) P(\mathcal{D}, x) - 1\right). \end{aligned} \tag{7.5}$$

The characters of all other building blocks for the EFT can be found in Ref. [64]. We will fix the exact spurion content and some other conventions in Sec. 7.2.2.

Because we also want to study CP effects in the EFT of ALPs, we have to discuss how to implement the action of CP on the ALP in terms of characters. In Sec. 2.5.2, we have presented how to include C and P transformations for the remaining fields appearing in the EFT. However, since the ALP is a singlet under the SM gauge group, the previous discussion no longer holds true and, in particular, the terms in the odd powers of the plethystic exponential of characters, which were vanishing for the SM fields due to their behaviour under C transformations, are non-vanishing for the ALP. The characters of the non-shift-symmetric and shift-symmetric axions appearing in odd powers of the Hilbert series are given by

$$\chi_a^-(\mathcal{D}, x) = \chi_a^{P^-}(\mathcal{D}, \tilde{x}) = -\mathcal{D}\left(1-\mathcal{D}^2\right) P_-(\mathcal{D}, \tilde{x}), \tag{7.6}$$

$$\chi_{\partial a}^-(\mathcal{D}, x) = \chi_{\partial a}^{P^-}(\mathcal{D}, \tilde{x}) = -\mathcal{D}\left(\left(1-\mathcal{D}^2\right) P_-(\mathcal{D}, \tilde{x}) - 1\right), \tag{7.7}$$

[1] For the construction of a Green's basis, the tower of EOM-redundant terms in $R_{\partial a}$ has to be kept in the calculation of the character. It corresponds to the negative term in the first line of Eq. (7.5). Without the subtraction of the EOM redundancy, the character for the Green's basis is given by $\chi_{\partial a}(\mathcal{D}, x) = \mathcal{D}(P(\mathcal{D}, x) - 1)$.

where P_{-} is defined in Eq. (2.117) and an overall minus sign was introduced to capture the pseudo-scalar nature of the axion under P transformations. The even-power characters are given in Eq. (2.110) and Eq. (7.5) respectively with where $P(\mathcal{D},x)$ has to be replaced with $P_{+}(\mathcal{D},\bar{x}) = P(\mathcal{D},\bar{x})$.

7.2.2 Conventions

As motivated in the introduction, we want to construct operator bases for the ALP EFTs above and below the EW scale, i.e. we will consider both the SMEFT and LEFT extended with an ALP, which we will refer to as aSMEFT and aLEFT in the following. Depending on the fate of the shift symmetry (or correspondingly the PQ symmetry) in the EFT, we define four EFTs with different spurion contents

- aSMEFT$_{\text{PQ}}$: SMEFT extended with a shift-symmetric axion
$$\{\mathcal{D},\partial a,Q,Q^\dagger,L,L^\dagger,H,H^\dagger,u,u^\dagger,d,d^\dagger,e,e^\dagger,B_L,B_R,W_L,W_R,G_L,G_R\}\,,$$
- aSMEFT$_{\not{\text{PQ}}}$: SMEFT extended with a non-shift-symmetric axion
$$\{\mathcal{D},a,Q,Q^\dagger,L,L^\dagger,H,H^\dagger,u,u^\dagger,d,d^\dagger,e,e^\dagger,B_L,B_R,W_L,W_R,G_L,G_R\}\,,$$
- aLEFT$_{\text{PQ}}$: LEFT extended with a shift-symmetric axion
$$\{\mathcal{D},\partial a,u_L,u_L^\dagger,u_R,u_R^\dagger,d_L,d_L^\dagger,d_R,d_R^\dagger,e_L,e_L^\dagger,e_R,e_R^\dagger,\nu_L,\nu_L^\dagger,F_L,F_R,G_L,G_R\}\,,$$
- aLEFT$_{\not{\text{PQ}}}$: LEFT extended with a non-shift-symmetric axion
$$\{\mathcal{D},a,u_L,u_L^\dagger,u_R,u_R^\dagger,d_L,d_L^\dagger,d_R,d_R^\dagger,e_L,e_L^\dagger,e_R,e_R^\dagger,\nu_L,\nu_L^\dagger,F_L,F_R,G_L,G_R\}\,.$$

Here, we follow the conventions of Ref. [85] by adding only left-handed Weyl fermions, living in the $\left(\frac{1}{2},0\right)$ representation of the Lorentz group, to the Hilbert series, also for the right-handed SM fermion, for which we drop the superscript "c" $u^c_{(R)}, d^c_{(R)}, e^c_{(R)} \in \left(\frac{1}{2},0\right)$ in the computation of the Hilbert series for brevity. For the field strengths $X = F, B, W, G$ we use the chiral components $X^{\mu\nu}_{L,R} = \frac{1}{2}(X^{\mu\nu} \pm i\tilde{X}^{\mu\nu})$, which excite a gauge boson of helicity ± 1 and hence, transform as $(1,0)$ and $(0,1)$ under the Lorentz group, respectively. The axion field transforms as a singlet under the Lorentz and SM gauge group, but transforms with a sign under parity transformations as was discussed in the last section.

For the computation of aSMEFT$_{\not{\text{PQ}}}$ the Haar measures and characters for all spurions that we just presented can be found in Ref. [85] and the full Hilbert series can be directly computed from Eq. (2.112). The only difference compared to the SMEFT lies in the inclusion of the axion field a, which is achieved by adding an additional PE for the spurion a in the calculation of the Hilbert series. For aSMEFT$_{\text{PQ}}$, we only need to change the spurion a to ∂a, and adopt the character in Eq. (7.5), after which the calculation of the Hilbert series will also be straightforward.

For the EFT below the EW scale, all left-handed and right-handed fermion fields are completely independent as a UV completion could be chiral (LEFT captures both SMEFT- and HEFT-like UV completions). The $SU(2)_L \times U(1)_Y$ part of the SM gauge group is broken to $U(1)_{\text{em}}$, whose charges are given by $Q = Y + T_3$. The calculation of the Hilbert series of

aLEFT_{PQ} and $\text{aLEFT}_{\not{\text{PQ}}}$ follows the same fashion as for the EFT above the EW scale, except that we need not integrate over the $SU(2)$ group, simplifying the calculations further. As for the aSMEFT, we have to use the appropriate spurions ∂a and a with their the corresponding character to capture the shift symmetry of the ALP correctly.

At low energies, the EFT with quarks and gluons as degrees of freedom eventually has to be matched to the chiral Lagrangian of QCD, in order to properly describe phenomena like exotic meson decays with final states including axions. Therefore, we also want to briefly comment on how to construct the Hilbert series for the QCD chiral Lagrangian extended with an axion. Following the analysis in Ref. [227], one would have to define two Cartan forms u_μ^{ALP} and u_μ^{QCD}, where u_μ^{ALP} as defined in Eq. (7.3) describes the ALP degrees of freedom and u_μ^{QCD} describes the low-energy QCD degrees of freedom. In contrast to u_μ^{ALP}, u_μ^{QCD} transforms under an internal $SU(N_f)_V$ symmetry, as low-energy QCD with N_f light flavours has the more involved symmetry breaking pattern $SU(N_f)_L \times SU(N_f)_R \to SU(N_f)_V$. Therefore, the character for u_μ^{QCD} has to be multiplied by the character of the adjoint of $SU(N_f)$ with respect to u_μ^{ALP} [227]. With the resulting Hilbert series, all operators for the QCD chiral Lagrangian can be easily constructed. If operators which break the shift-symmetry of the ALP are also of interest, a pseudoscalar with the character given by Eq. (2.110) has to be added to the Hilbert series along u_μ^{QCD}.

Since, we want to construct the EFT order by order in the EFT expansion, it is convenient to grade the fields in the mass dimension. This will allow us to easily truncate the Hilbert series at the right order. For this, we will rescale the spurions with their mass dimensions $\phi \to \epsilon\phi$ for scalars, $\psi \to \epsilon^{3/2}\psi$ for fermions, $X \to \epsilon^2 X$ for field strengths, $\partial a \to \epsilon^2 \partial a$ and $\mathcal{D} \to \epsilon\mathcal{D}$ for the covariant derivative. We define the graded Hilbert series as $\mathcal{H}(\epsilon) = \sum_i \epsilon^i \mathcal{H}_i$. It should be noted that the calculation of the full Hilbert series is impossible. However, in the construction of the operator basis, it suffices to focus only on a specific mass dimension.

The computation of the Hilbert series can be significantly simplified by always truncating terms appearing in the integrand of Eq. (2.112) as early as possible in the mass dimension. In practice, this means that we expand PE/P to the desired mass dimension first and then perform the integration over the Haar measures. Nevertheless, expanding the integrand itself becomes challenging at higher mass dimensions. To address this, a FORM code called ECO (Efficient Counting of Operators) [302] has been developed specifically for efficient Hilbert series calculation. For this project, the Mathematica code `CHINCHILLA` was developed, which efficiently computes the Hilbert series by cleverly expanding the integrand of the Hilbert series. The code will be published in a forthcoming paper [260].

7.3 aSMEFT

We are now ready to calculate the Hilbert series and construct all operators of the SMEFT extended with a light pseudoscalar. We will start with an ALP, i.e., a pseudoscalar with a shift symmetry, stemming from its Goldstone boson nature under the spontaneously broken global $U(1)_{\text{PQ}}$ symmetry.

7.3.1 aSMEFT$_{\mathbf{PQ}}$

Using the tools introduced in Sec. 2.5.2 and the spurion content defined in Sec. 7.2.2, we will first compute the Hilbert series of the EFT with a derivatively coupled pseudoscalar ∂a. Evaluating Eq. (2.112) for the given spurions, we find the Hilbert series for one generation of fermions up to mass dimension 8 to be[2]

$$\begin{aligned}
\mathcal{H}_5^{\text{PQ}} &= \partial a\, QQ^\dagger + \partial a\, uu^\dagger + \partial a\, dd^\dagger + \partial a\, LL^\dagger + \partial a\, ee^\dagger + \partial a\, HH^\dagger \mathcal{D} \\
&\quad - \partial a\, B_L \mathcal{D} - \partial a\, B_R \mathcal{D} - \partial a\, \mathcal{D}^3 , \\
\mathcal{H}_6^{\text{PQ}} &= (\partial a)^2 HH^\dagger , \\
\mathcal{H}_7^{\text{PQ}} &= \partial a\, QQ^\dagger B_L + \partial a\, QQ^\dagger B_R + \partial a\, QQ^\dagger G_L + \partial a\, QQ^\dagger G_R + \partial a\, QQ^\dagger W_L + \partial a\, QQ^\dagger W_R \\
&\quad + \partial a\, uu^\dagger B_L + \partial a\, uu^\dagger B_R + \partial a\, uu^\dagger G_L + \partial a\, uu^\dagger G_R + \partial a\, dd^\dagger B_L + \partial a\, dd^\dagger B_R \\
&\quad + \partial a\, dd^\dagger G_L + \partial a\, dd^\dagger G_R + \partial a\, LL^\dagger B_L + \partial a\, LL^\dagger B_R + \partial a\, LL^\dagger W_L + \partial a\, LL^\dagger W_R \\
&\quad + \partial a\, ee^\dagger B_L + \partial a\, ee^\dagger B_R + 2\partial a\, QQ^\dagger HH^\dagger + \partial a\, uu^\dagger HH^\dagger + \partial a\, dd^\dagger HH^\dagger \\
&\quad + 2\partial a\, LL^\dagger HH^\dagger + \partial a\, ee^\dagger HH^\dagger + \partial a\, B_L HH^\dagger \mathcal{D} + \partial a\, B_R HH^\dagger \mathcal{D} + \partial a\, W_L HH^\dagger \mathcal{D} \\
&\quad + \partial a\, W_R HH^\dagger \mathcal{D} + \partial a\, H^2 H^{\dagger 2} \mathcal{D} + 2\partial a\, QuH\mathcal{D} + 2\partial a\, Q^\dagger u^\dagger H^\dagger \mathcal{D} + 2\partial a\, QdH^\dagger \mathcal{D} \\
&\quad + 2\partial a\, Q^\dagger d^\dagger H\mathcal{D} + 2\partial a\, LeH^\dagger \mathcal{D} + 2\partial a\, L^\dagger e^\dagger H\mathcal{D} , \\
\mathcal{H}_8^{\text{PQ}} &= (\partial a)^4 + (\partial a)^2 QQ^\dagger \mathcal{D} + (\partial a)^2 uu^\dagger \mathcal{D} + (\partial a)^2 dd^\dagger \mathcal{D} + (\partial a)^2 LL^\dagger \mathcal{D} + (\partial a)^2 ee^\dagger \mathcal{D} \\
&\quad + (\partial a)^2 B_L^2 + (\partial a)^2 B_L B_R + (\partial a)^2 B_R^2 + (\partial a)^2 G_L^2 + (\partial a)^2 G_L G_R + (\partial a)^2 G_R^2 \\
&\quad + (\partial a)^2 W_L^2 + (\partial a)^2 W_L W_R + (\partial a)^2 W_R^2 + \partial a\, Qd^{\dagger 2} L^\dagger + \partial a\, Q^\dagger d^2 L + \partial a\, ud^\dagger L^{\dagger 2} \\
&\quad + \partial a\, u^\dagger dL^2 + 2(\partial a)^2 HH^\dagger \mathcal{D}^2 + 2\partial a\, L^2 H^2 \mathcal{D} + 2\partial a\, L^{\dagger 2} H^{\dagger 2} \mathcal{D} + (\partial a)^2 H^2 H^{\dagger 2} \\
&\quad + (\partial a)^2 QuH + (\partial a)^2 Q^\dagger u^\dagger H^\dagger + (\partial a)^2 QdH^\dagger + (\partial a)^2 Q^\dagger d^\dagger H + (\partial a)^2 LeH^\dagger \\
&\quad + (\partial a)^2 L^\dagger e^\dagger H .
\end{aligned} \tag{7.8}$$

Every term in the Hilbert series can be interpreted as an effective operator with the field content given by the spurions and the prefactor counting the number of operator with that field content. For instance, for the first term in $\mathcal{H}_5^{\text{PQ}}$, we expect a single operator with the field content $\partial_\mu a, Q, Q^\dagger$. Using this this information, it is straightforward to write down a gauge- and Lorentz-invariant operator $\partial_\mu a\, \bar{Q}\gamma^\mu Q$.

The negative terms appearing at dimension 5 do not correspond to non-redundant operators and are cancelled exactly by other terms in $\Delta\mathcal{H}$, which can be computed immediately from the expression of $\Delta\mathcal{H}$ given in Ref. [64]. Evaluating the expression, we find for the terms containing an ALP field[3]

$$\Delta\mathcal{H} = \partial a\, B_L \mathcal{D} + \partial a\, B_R \mathcal{D} + \partial a\, \mathcal{D}^3 , \tag{7.9}$$

[2] Note that $\mathcal{H}_5^{\text{PQ}}$ here only corresponds to the first term in Eq. (2.112) and we still have to add $\Delta\mathcal{H}$, which is non-trivial here, to get the correct full result. Furthermore, we have only kept the axion-dependent terms.

[3] Note, that the $\mathcal{D}^4$ term that usually appears in $\mathcal{H}_0$ and is cancelled by a term in $\Delta\mathcal{H}$ does not appear here because we only keep terms in the Hilbert series which include at least on ALP field a.

which exactly cancel the negative terms in $\mathcal{H}_0$. The form of the terms is similar to those found in the discussion of the QCD chiral Lagrangian in Ref. [227], where a more involved case of a non-linearly realised symmetry is analysed. The only difference to our analysis lies in the counting of the mass dimension of the field spurions capturing the Goldstone degrees of freedom. As mentioned in the last section, because of the simple symmetry breaking pattern under which the ALP arises as the Goldstone boson, we have simplified $u_\mu = i\frac{\partial_\mu a}{f}$ where we put the $1/f$ suppression into the Wilson coefficient. Hence, in our case $[\partial a] = 2$, whereas usually $[u_\mu] = 1$. That is why $\Delta\mathcal{H}$ gets ALP-dependent contributions at dimension-5 here, whereas usually it only has terms of mass dimension 4. For instance, terms like $u\,B_L\mathcal{D} \sim \partial a\,B_L\mathcal{D}$ appear at dimension 5 here. The last term in Eq. (7.9) can only appear here due to the gauge-singlet nature of the ALP, while the other two terms are also generated for non-Abelian gauge groups if the scalar transforms in the adjoint representation.

For brevity, the Hilbert series in Eq. (7.8) only takes one flavour of fermions into account, which is enough to construct most operators. However, in some cases multiple flavours are necessary for certain operator structures to be non-vanishing and the above Hilbert series is not enough to construct the operator basis. To compute the Hilbert series for a general number of flavours N_f, N_f copies of the corresponding fermions' PE have to be added in the Molien-Weyl formula, which is equivalent to simply adding a factor of N_f in front of the fermionic part of the PE (c.f. Eq. (2.102)). Indeed, looking at the dimension-8 Hilbert series for generic N_f, we find the following terms

$$\mathcal{H}_8^{\rm PQ} \supset \frac{1}{3}N_f^2\left(N_f^2-1\right)\partial a\,d^{\dagger 3}e + \frac{1}{3}N_f^2\left(N_f^2-1\right)\partial a\,d^3 e^\dagger\,, \tag{7.10}$$

which evidently vanish for $N_f = 1$. These terms can only appear for $N_f > 1$ because of the antisymmetric colour structure of the down quarks in the corresponding operator which only gives rise to a non-vanishing operator if the down-type quarks come in at least two different flavours (c.f. operator $\mathcal{O}_{\partial aed}$ in Tab. 7.6).

Even after adding ΔH to the Hilbert series in Eq. (7.8), it still does not quite give the correct number of non-redundant operators and some further adjustments have to be performed. First of all, the redundant operator $\mathcal{O}_{\partial aH} = \partial^\mu a\left(H^\dagger i\overleftrightarrow{D}_\mu H\right)$ corresponding to the term $\partial a\,HH^\dagger\mathcal{D}$ in $\mathcal{H}_5^{\rm PQ}$ is not removed automatically.[4] This is due to the fact that the operator can be removed by a global hypercharge transformation on the Higgs field which we have not implemented into the Hilbert series. As discussed in Sec. 2.4.3, all derivative couplings of the ALP to SM particles are only defined up to redefinitions by exact global symmetries. We have not imposed the condition $\partial_\mu j^\mu = 0$ for conserved currents in our approach, which as discussed in Sec. 2.4.3 can remove operators with derivatively coupled classically conserved currents $\partial_\mu a\, j^\mu$ from the EFT. In principal, we could remove redundancies of the form $\partial_\mu j^\mu = 0$ using an appropriate shortening condition for a conformal character as was done to remove the EOM redundancies [64]. In order to do this, one would have to use the conserved currents

[4] We can check that this does not happen again at higher mass dimensions using Eq. (7.20). Without imposing a shift symmetry any operator that exactly gives an EOM-redundant operator upon using IBP will be removed because one derivative is no longer fixed to the ALP by demanding derivatively coupled ALP interactions.

themselves as building blocks in the Hilbert series. This is impractical in our case, because all fermions obviously not only come in the form of such currents and hence, it is easier to just remove such redundancies by hand at the end.

Secondly, there are the anomalous operators of the form $aF\widetilde{F}$ at mass dimension 5 which do not appear in the Hilbert series. This is because we use ∂a as a building block to directly impose the shift symmetry of the ALP. One can easily show by moving the derivative from the first field strength by IBP to the ALP that this operator is shift-symmetric (up to non-perturbative effects). Then however, the gauge field A_μ appears by itself and we would have to use the gauge fields themselves as a building block which is practically unfeasible with the Hilbert series, and would also be inconvenient from the perspective of constructing gauge-invariant operators. To include these operators systematically, it will prove useful that we also build an operator basis for an ALP without a shift symmetry in Section 7.3.2, where we use just a as a building block. Noticing that the $aF\widetilde{F}$-type operators will remain after taking the shift-symmetric limit we have a way of taking these operators into account.

For most terms in the Hilbert series shown in Eq. (7.8) it is straightforward to build Lorentz- and gauge-invariant operators from the spurion content and get the correct number of independent operators as indicated by the Hilbert series. There is one exception that is a bit more involved, the operators of type $(\partial a)^2 X^2$ at dimension 8. From the Hilbert series in Eq. (7.8), we can read off that we should expect three non-redundant operators $X_L^2(\partial a)^2$, $X_L X_R(\partial a)^2$ and $X_R^2(\partial a)^2$. However, one can naively build 4 operators

$$\partial_\mu a \partial^\mu a\, B_{\nu\rho} B^{\nu\rho}, \quad \partial_\mu a \partial^\mu a\, B_{\nu\rho} \widetilde{B}^{\nu\rho}, \quad \partial_\mu a \partial^\nu a\, B^{\mu\rho} B_{\nu\rho}, \quad \partial_\mu a \partial^\nu a\, B^{\mu\rho} \widetilde{B}_{\nu\rho} \tag{7.11}$$

sharing a complicated relation that renders one of the operators redundant. We can use the Schouten identity (see e.g. Ref. [306])

$$g_{\mu\nu}\epsilon_{\alpha\beta\gamma\delta} + g_{\mu\alpha}\epsilon_{\beta\gamma\delta\nu} + g_{\mu\beta}\epsilon_{\gamma\delta\nu\alpha} + g_{\mu\gamma}\epsilon_{\delta\nu\alpha\beta} + g_{\mu\delta}\epsilon_{\nu\alpha\beta\gamma} = 0 \tag{7.12}$$

to relate the two operators with a dual field strength. Contracting the indices in the identity with a generic rank-2 tensor $T^{\mu\nu}$ (which we identify with $\partial^\mu a \partial^\nu a$) and an anti-symmetric rank-2 tensor $X_{\mu\nu}$ yields

$$T_{\mu\nu} X^{\mu\rho} \widetilde{X}^{\nu}{}_{\rho} = \frac{1}{4} T^\mu_\mu X_{\nu\rho} \widetilde{X}^{\nu\rho} \tag{7.13}$$

explaining the number of operators of that type in the Hilbert series. Our complete basis up to mass dimension 8 can be found in Tabs. 7.3, 7.4, 7.5 and 7.6 in App. 7.A.1.

There are several ways to cross-check our results. As a sanity check for our implementation of the Hilbert series we can use the a^0 terms to compare our results for the Hilbert series with Ref. [85] and the operators with the SMEFT operator basis up to dimension 8 [63, 87–89].

Furthermore, some results for the ALP EFT are available in the literature up to dimension 7. Our results at dimension 5 are consistent with the usual basis at dimension 5 (see e.g. Ref. [175]). The results at dimension 6 are consistent with Ref. [176, 196, 296, 297]. Some results at dimension 7 can be found in Ref. [196, 298] and are consistent with our operator basis. More results for higher-dimensional operators can be found in Ref. [194] where the authors match some of the operators in the chiral electroweak EFT extended with an axion to the one in a linear realisation. All operators they find are either in our basis or equivalent to operators in our basis due to field redefinitions and IBP.

It is also rather straightforward to construct the Hilbert series for a Green's basis of the ALP EFT by using the characters computed with the long representations that include EOM redundancies. A complete discussion is beyond the scope of this work. Instead, we show a simple example of the Hilbert series at dimension 6 for the Green's basis. After the characters for the long representations are used as an input for the Hilbert series, it can be computed just like for the EOM-reduced single particle modules. The dimension-6 Hilbert series takes the following form

$$\mathcal{H}_6^{\mathrm{PQ}} = (\partial a)^2 H H^\dagger + (\partial a)^2 \mathcal{D}^2 \,. \tag{7.14}$$

Comparing with the dimension-6 Hilbert series in Eq. (7.8), the first term is the same as in the non-redundant basis, which correspond to the operator $\partial_\mu a \partial^\mu a |H|^2$, while the second term is an EOM-redundant term and corresponds to the operator $\partial^2 a \partial^2 a$. All other operators at higher mass dimensions can in principle be constructed in the same way using the Hilbert series as a guide.

To understand how the number of operators $\#\,\mathcal{O}_{d_i}^{\mathrm{PQ}}$ behaves as a function of the number of flavours at each mass dimension d_i, we set all field spurions in the Hilbert series with full flavour dependence to unity such that only the dependence on N_f remains. By furthermore rephasing all fermionic spurions with lepton number and baryon number transformations respectively, i.e. $\ell \to \epsilon_L \ell$, $\ell^\dagger \to \epsilon_L^{-1} \ell^\dagger$ and $q \to \epsilon_B^{1/3} q$, $q^\dagger \to \epsilon_B^{-1/3} q^\dagger$, we can in addition obtain the number of operators that break lepton and baryon number at each mass dimension. Then for each power of $\epsilon_{B,L}$ in the following expressions, baryon number and lepton number are violated by one unit. After taking care of the caveats we have mentioned above by hand, we find[5]

$$\begin{aligned}
\#\,\mathcal{O}_5^{\mathrm{PQ}} &= 2 - N_f + 5N_f^2 \,, \\
\#\,\mathcal{O}_6^{\mathrm{PQ}} &= 1 \,, \\
\#\,\mathcal{O}_7^{\mathrm{PQ}} &= 5 + 39N_f^2 \,, \\
\#\,\mathcal{O}_8^{\mathrm{PQ}} &= \left(13 + 11N_f^2\right) + \left(-\frac{2N_f^2}{3} + \frac{8N_f^4}{3}\right)\epsilon_B \epsilon_L + \left(4N_f^2 + 2N_f^4\right)\epsilon_L^2 \,, && (7.15) \\
& && (7.16)
\end{aligned}$$

The total number of operators is obtained by setting $\epsilon_{B,L} \to 1$. More results for the higher mass dimensions are shown in Ref. [2] and its ancillary material. Notice, that baryon and lepton number-breaking operators only appear at mass dimension 8. This is due to the derivative coupling of the ALP that only allows for baryon and lepton number-breaking terms through the coupling of $\partial_\mu a$ to 4-fermion operators.

[5] After all terms have been simplified, we make the replacement $\epsilon_i^{-n} \to \epsilon_i^n$, such that all operators breaking baryon and lepton number by a positive or negative value n w.r.t. the conserving case are counted in the same way.

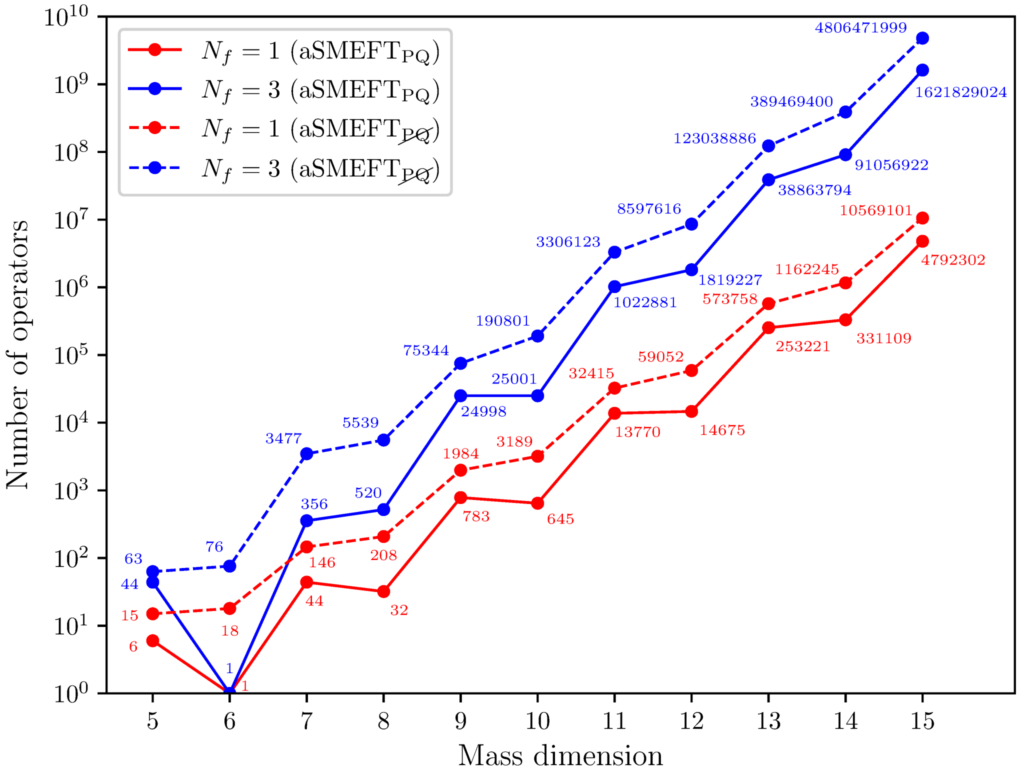


Figure 7.1: The number of operators in the aSMEFT with and without a shift symmetry for the ALP plotted against the mass dimension for $N_f = 1$ and $N_f = 3$ number of flavours.

In Fig. 7.1, we have plotted the number of operators of the ALP EFT up to mass dimension 15 for one and three flavours of fermions. It can be seen that the operators grow rapidly with the mass dimension as is common in effective theories [307]. There exist also some unusual features due to the derivative nature of the shift-symmetric ALP couplings. For instance, at dimension 6 there exists only a single operator. At higher mass dimensions on the other hand, the multiplicity of operators increases in the same manner as one is accustomed to from other EFTs.

7.3.2 aSMEFT$_{\not{\text{PQ}}}$

In this section, we will work out the difference between an ALP and a generic pseudoscalar. To this end, we relax the assumption of a shift symmetry for the pseudoscalar, which no longer necessarily has to be connected to the spontaneous breaking of a PQ symmetry. However, there can still be such a connection by assuming that the spontaneously broken global symmetry is only approximate. Then, all shift-breaking operators are understood as small corrections to those that conserve the shift symmetry and it is important to understand the limit of an exact shift symmetry.

As the shift symmetry is now relaxed, the field a itself is now the appropriate building block for the Hilbert series. As before, the Hilbert series is computed by evaluating Eq. (2.112) with the appropriate characters and Haar measures for the given field spurions and symmetries. For one generation of fermions we obtain up to mass dimension 7

$$
\begin{aligned}
\mathcal{H}_5^{\cancel{\text{PQ}}} =& a^5 + aB_L^2 + aB_R^2 + aG_L^2 + aG_R^2 + aW_L^2 + aW_R^2 + a^3 HH^\dagger + aH^2 H^{\dagger 2} + aQuH \\
&+ aQ^\dagger u^\dagger H^\dagger + aQdH^\dagger + aQ^\dagger d^\dagger H + aLeH^\dagger + aL^\dagger e^\dagger H \\
=& a\,\mathcal{H}_4^{\text{SM}} + a^5 + a^3 HH^\dagger \,, \\
\mathcal{H}_6^{\cancel{\text{PQ}}} =& a\,\mathcal{H}_5^{\cancel{\text{PQ}}} + aH^2L^2 + aH^{\dagger 2}L^{\dagger 2} + a^2 HH^\dagger \mathcal{D}^2 \,, \\
\mathcal{H}_7^{\cancel{\text{PQ}}} =& a\,\mathcal{H}_6^{\cancel{\text{PQ}}} + a\,\mathcal{H}_6^{\text{SMEFT}} + aQQ^\dagger B_L\mathcal{D} + aQQ^\dagger B_R\mathcal{D} + aQQ^\dagger G_L\mathcal{D} + aQQ^\dagger G_R\mathcal{D} \\
&+ aQQ^\dagger W_L\mathcal{D} + aQQ^\dagger W_R\mathcal{D} + auu^\dagger B_L\mathcal{D} + auu^\dagger B_R\mathcal{D} + auu^\dagger G_L\mathcal{D} + auu^\dagger G_R\mathcal{D} \\
&+ add^\dagger B_L\mathcal{D} + add^\dagger B_R\mathcal{D} + add^\dagger G_L\mathcal{D} + add^\dagger G_R\mathcal{D} + aLL^\dagger B_L\mathcal{D} + aLL^\dagger B_R\mathcal{D} \\
&+ aLL^\dagger W_L\mathcal{D} + aLL^\dagger W_R\mathcal{D} + aee^\dagger B_L\mathcal{D} + aee^\dagger B_R\mathcal{D} + 2aQQ^\dagger HH^\dagger\mathcal{D} \\
&+ auu^\dagger HH^\dagger\mathcal{D} + add^\dagger HH^\dagger\mathcal{D} + 2aLL^\dagger HH^\dagger\mathcal{D} + aee^\dagger HH^\dagger\mathcal{D} + aB_L HH^\dagger\mathcal{D}^2 \\
&+ aB_R HH^\dagger\mathcal{D}^2 + aW_L HH^\dagger\mathcal{D}^2 + aW_R HH^\dagger\mathcal{D}^2 + aH^2H^{\dagger 2}\mathcal{D}^2 + 2aQuH\mathcal{D}^2 \\
&+ 2aQ^\dagger u^\dagger H^\dagger\mathcal{D}^2 + 2aQdH^\dagger\mathcal{D}^2 + 2aQ^\dagger d^\dagger H\mathcal{D}^2 + 2aLeH^\dagger\mathcal{D}^2 + 2aL^\dagger e^\dagger H\mathcal{D}^2 \,.
\end{aligned}
\tag{7.17}
$$

At dimension 5, there exists no term where the ALP is derivatively coupled to fermions corresponding to $\mathcal{H}_5^{\text{PQ}}$ computed previously. We have[6]

$$
\mathcal{H}_5^{\cancel{\text{PQ}}} = a\mathcal{H}_4^{\cancel{\text{PQ}}} + a\mathcal{H}_4^{\text{SM}} \,, \tag{7.18}
$$

which is the well-known result that, at dimension 5, the fermionic operators with the derivatively coupled ALP are redundant by the EOM [176, 194, 212, 213] and can be projected on the ALP-Yukawa operators. Hence, only keeping the ALP-Yukawa operators is sufficient to capture both shift-breaking and shift-preserving terms. Allowing for the lepton number-breaking Weinberg operator in the dimension-5 SMEFT, we find the following relation at the level of the Hilbert series

$$
\mathcal{H}_6^{\cancel{\text{PQ}}} = a\,\mathcal{H}_5^{\cancel{\text{PQ}}} + a\,\mathcal{H}_5^{\text{SMEFT}} + \mathcal{H}_6^{\text{PQ}}\left(\partial a \to a\mathcal{D}\right) \,. \tag{7.19}
$$

Here, $\mathcal{H}_i^{\cancel{\text{PQ}}}$ is the Hilbert series of the ALP EFT with a as a building block, $\mathcal{H}_i^{\text{SMEFT}}$ is the Hilbert series of the SMEFT and $\mathcal{H}_6^{\text{PQ}}$ is the Hilbert series of the ALP EFT with ∂a as a building block, each at mass dimension i. The expression in the bracket is understood as replacing the spurion ∂a of the derivatively coupled ALP with the ALP spurion a and the spurion of the covariant derivative $\mathcal{D}$. This simplifies identifying the explicitly shift-symmetric derivatively coupled interactions between the ALP and the SM particles.

We conjecture that this relation at the level of the Hilbert series holds true at any mass dimension beyond dimension 5.[7] In general, we conjecture that the Hilbert series fulfils the

[6] Here, $\mathcal{H}_4^{\text{SM}}$ does not contain the kinetic term of fermions and scalars, because they are proportional to the EOM [64].

[7] We have checked explicitly that this separation appears up to mass dimension 15 and believe that it

following condition at mass dimension n

$$\mathcal{H}_n^{\text{P}\!\!\!\!\text{Q}} = a\,\mathcal{H}_{n-1}^{\text{P}\!\!\!\!\text{Q}} + a\,\mathcal{H}_{n-1}^{\text{SMEFT}} + \mathcal{H}_n^{\text{PQ}}(\partial a \to a\mathcal{D})\,, \qquad n > 5 \tag{7.20}$$

which we have verified to hold true up to $n = 15$. In the following, we will refer to this relation as the *Peccei–Quinn breaking isolation condition* or *shift-breaking isolation condition*. We want to emphasise the importance of this equation. It states that above dimension 5 the EFT splits into a part generated by simply multiplying the operators at the previous mass dimension with an ALP field – which immediately follows from the singlet scalar nature of the ALP – and a second part which is exactly the EFT built with a derivatively coupled, i.e. explicitly shift-invariant ALP. This separation of the shift-breaking and shift-symmetric sectors of the ALP EFT can be captured with the Hilbert series in a concise way. We will explore the implications of this further in Section 7.3.3.

Constructing the operators for the shift-breaking interactions of the ALP is trivial, as the ALP is a singlet both under the Lorentz and the gauge group. Then, any gauge- and Lorentz-invariant operator can be multiplied by an ALP to receive a new Lorentz invariant operator. Following Eq. (7.20), it can be seen that, by this construction, a complete operator basis is obtained after adding the derivatively coupled terms that we have constructed in Section 7.3.1.

Our complete basis for an ALP without a shift symmetry coupled to the SM particles at mass dimension 5 can be found in Tab. 7.7 and the operator bases up to mass dimension 8 can be constructed easily with the shift-breaking isolation condition (see App. 7.A.2 for details). Since a potential can be written down for the ALP after relaxing its shift symmetry, we will also show the renormalisable part of the Lagrangian here listing the remaining terms we have not constructed thus far. The renormalisable Lagrangian is given by

$$\mathcal{L}^a_{\leq 4} = \frac{1}{2}\partial_\mu a\,\partial^\mu a - \frac{m_{a,0}^2}{2}\,a^2 + C_{a^3}\,a^3 + C_{a^4}\,a^4 + C_{aH^2}\,a\,|H|^2 + C_{a^2H^2}\,a^2|H|^2\,. \tag{7.21}$$

To cross-check the completeness of our operator basis, we have compared it with the operator bases of Refs. [276, 308] and find agreement for the terms breaking the shift symmetry.

As before, we can obtain expressions for the number of operators as a function of the number of fermion generations at each mass dimension by setting all spurions to unity. We find

$$\#\,\mathcal{O}_5^{\text{P}\!\!\!\!\text{Q}} = 9 + 6N_f^2\,,$$
$$\#\,\mathcal{O}_6^{\text{P}\!\!\!\!\text{Q}} = \left(10 + 6N_f^2\right) + \left(N_f + N_f^2\right)\epsilon_L^2\,,$$

---

holds also true for all higher order operators. To get a redundancy like at dimension 5, an operator with a derivatively coupled axion has to fulfil an EOM relation upon moving the derivative from the axion to the rest of the operator using IBP. As the operators become more and more complicated for higher mass dimensions, it is less and less likely that through this procedure a structure is obtained which exactly resembles the EOM of an SM particle as at dimension 5.

$$\#\,\mathcal{O}_7^{\not{\rm PQ}} = \left(30 + \frac{315N_f^2}{4} + \frac{N_f^3}{2} + \frac{107N_f^4}{4}\right) + \left(\frac{2N_f^2}{3} + N_f^3 + \frac{19N_f^4}{3}\right)\epsilon_B\epsilon_L + \left(N_f + N_f^2\right)\epsilon_L^2\,,$$
$$\#\,\mathcal{O}_8^{\not{\rm PQ}} = \left(43 + \frac{359N_f^2}{4} + \frac{N_f^3}{2} + \frac{107N_f^4}{4}\right) + \left(3N_f + \frac{41N_f^2}{3} + N_f^3 + \frac{37N_f^4}{3}\right)\epsilon_L^2 + \left(2N_f^3 + 16N_f^4\right)\epsilon_B\epsilon_L\,. \tag{7.22}$$

In the case of a generic pseudoscalar, lepton number-violating terms already appear at dimension 6, whereas for a shift-symmetric ALP lepton and baryon number-violating terms only appear at dimension 8. This is because the ALP no longer has to be derivatively coupled, and can for instance simply multiply the Weinberg operator of the SMEFT to give a lepton number violating operator at dimension 6. More results can be found in Ref. [2].

In Fig. 7.1, we have also plotted the number of operators against the mass dimension for the SMEFT extended with an ALP without a shift symmetry. Since new singlets under the gauge and Lorentz group can trivially be built by multiplying operators appearing at earlier mass dimension by the ALP field a once the shift symmetry is relaxed (c.f. Eq. (7.20)), the total number of operators counted by the Hilbert series increases steadily with the mass dimension. Comparing the number of operators at dimension 5 between the explicitly shift-symmetric and non-shift-symmetric Lagrangian in Fig 7.1, the difference $63 - 44 = 19$ corresponds exactly to the number of shift-breaking invariants (13) constructed in Chap. 6 plus the number of conditions that have to be imposed on the bosonic shift symmetry breaking operators (6) (c.f. Tab. 7.7). We will discuss the shift-symmetric limit in more details in Section 7.3.3.

7.3.3 Taking the Shift-Symmetric Limit

We have already discussed the implications of the EOM redundancy in the ALP EFT at dimension 5 in Sec. 2.4.3 and Chap.ch:ALPEFTShS. To properly take the shift-symmetric limit, the Wilson coefficients of the dimension-5 fermionic operator EFT of a generic pseudoscalar[8]

$$\mathcal{L}^a = -\bar{L}Y_eHe - \bar{Q}Y_u\tilde{H}u - \bar{Q}Y_dHd + \frac{a}{f}\left(\bar{L}C_{ae}He + \bar{Q}C_{au}\tilde{H}u + \bar{Q}C_{ad}Hd\right) + \text{h.c.}\,. \tag{7.23}$$

have to take the following form to describe a shift-symmetric ALP

$$C_{au} = i\left(C_QY_u - Y_uC_u\right),\ C_{ad} = i\left(C_QY_d - Y_dC_d\right),\ C_{ae} = i\left(C_LY_e - Y_eC_e\right)\,. \tag{7.24}$$

These matrix relations lead to difficulties in the interpretation of the shift symmetry in the EFT picture because the same operator has to capture physics corresponding to the shift-breaking and shift-symmetric sector which usually arise at very different scales. Furthermore, taking the shift-symmetric limit in the EFT where one uses a as a building block requires some care. This is resolved by the 13 order parameters for shift symmetry constructed in Chap. 6, allowing to implement the different power countings of the shift-breaking and shift-conserving

[8] Here, we have introduced new notation for the Wilson coefficients to make the conventions for the operator basis later more systematic.

sector in a straightforward way. From now on, we will refer to the Lagrangian in Eq. (7.23) as the Yukawa basis given that the relations in Eq. (7.24) are fulfilled.

We will now explore if similar relations, that have to be imposed in order to take the shift-symmetric limit, exist in the non-shift-symmetric EFT at higher mass dimensions using the operator basis we have derived above. The first observation we want to make is based on the Peccei–Quinn breaking isolation condition in Eq. (7.20). For $n > 5$ we have found previously

$$\mathcal{H}_n^{\not{PQ}} = a\,\mathcal{H}_{n-1}^{\not{PQ}} + a\,\mathcal{H}_{n-1}^{\text{SMEFT}} + \mathcal{H}_n^{\text{PQ}}\,(\partial a \to a\mathcal{D})\ . \tag{7.25}$$

The Hilbert series which is obtained by imposing the shift symmetry explicitly, $\mathcal{H}_n^{\text{PQ}}$, appears fully in the Hilbert series of the theory where a itself is used as a spurion. This implies that beyond dimension 5 no further EOM redundancies appear and all operator structures stay non-redundant in the presence of shift-breaking interactions. Therefore, if one decides to work in the operator basis with derivatively coupled interactions at dimension-5, all shift-symmetric couplings are exactly captured by the derivative interactions.

This is however only true in the operator basis, where the ALP is derivatively coupled to the fermions at dimension 5. One has to be more careful when working in the Yukawa basis, which is the more natural basis in the presence of shift-breaking effects as we will comment on below. Here, care has to be taken while removing the EOM redundancy at dimension 5 when higher-order operators are considered in the EFT. To remove the redundancy at dimension 5 in the presence of higher dimensional operators, field redefinitions have to be used instead of simply plugging in the classical EOM of the fields to remove the derivatively coupled operators at dimension 5 and all terms generated by the field redefinitions up to the considered order in the EFT have to be kept. We have done this carefully in App. 7.C, where we find that the field redefinition removing the EOM redundancy at dimension 5 indeed generates more (seemingly shift-breaking) operators whose Wilson coefficients are fully constrained by relations similar to those in Eq. (7.24) restoring shift symmetry in the EFT.

It is important to keep track of this at higher mass dimensions, as in the Yukawa basis the same operator captures shift-breaking and shift-preserving effects, which can come with very different suppression as the spontaneous and explicit breaking of the PQ symmetry usually arise at very different scales. To implement the power counting correctly for both sectors, flavour invariants acting as order parameters for the ALP shift symmetry as presented in Ch. 6 should be constructed for the matrix relations of the higher order operators generated by the field redefinition removing the EOM redundancy at dimension 5.

These matrix relations should also be kept in mind while taking the shift-symmetric limit going from the EFT of a generic pseudoscalar to the EFT of a shift-symmetric scalar in the Yukawa basis. Instead of setting all non-derivatively coupled operators to zero, one should set them to the constrained form that is found applying the appropriate field redefinitions. Alternatively, after constructing the flavour invariants one can simply perform the computation without keeping the shift symmetry in mind and express the final result in terms of the invariants. Then, it is straightforward to identify the shift-breaking and shift-preserving contributions.

Note that the Yukawa basis is in some sense the more natural basis to perform this limit, because the EFT of a generic pseudoscalar only contains the Yukawa couplings of the pseudoscalar to the SM fermions, but not the derivatively coupled interactions due to the EOM redundancy. Working in the shift-symmetric EFT in the Yukawa basis allows to directly take the shift-symmetric limit or compare the couplings in the case of a weakly broken shift symmetry. If one were to work in the derivatively coupled basis instead, there is no direct way to map or compare the shift-breaking couplings of the EFT of the generic pseudoscalar to those of the shift-symmetric scalar. We discuss further relations that have to be imposed besides those presented in Eq. (7.24) in App. 7.C.3, where we perform the necessary field redefinitions to go from one basis to the other while carefully keeping track of all generated terms up to the necessary mass dimensions.

The additional constrained interactions are crucial for explicit calculations in the Yukawa basis. If the additional terms are not included, one will run into results in the shift-symmetric EFT in the Yukawa basis which are not shift-invariant. E.g. if two insertions of the dimension-5 ALP-Yukawa couplings are considered, one must also add the diagram with the constrained interaction of the dimension-6 ALP-Yukawa coupling (see for instance Refs. [309–311] for recent studies, where these effects where correctly taken into account). Note that up to dimension-7 only the ALP-Yukawa operators with higher powers of the ALPs have to be considered and only starting at dimension-8, more operators with constrained Wilson coefficients are generated by the field redefinition. In addition, because ALP-dependent field redefinitions on the SM fermions are applied to change the operator basis, also SMEFT operators are affected by these field redefinitions, which first appear at dimension 7 for a lepton number-conserving SMEFT. Therefore, if mixed SMEFT–ALP EFT corrections are computed, those effects also have to be taken into account to preserve the shift symmetry up to the given order in the EFT.

It is also instructive, to perform the analysis with on-shell amplitudes [312] by imposing Adler's zero condition [313, 314]. Here, by carefully imposing Adler's zero condition the well-known conditions on the dimension-5 couplings and more relations at higher mass dimensions are found, consistent with our analysis with the Hilbert series and field redefinitions. In the on-shell approach, these relations can be understood from fundamental properties of amplitudes like analyticity and regularity of the amplitude in the limit of soft ALP momenta (for details see Ref. [312]).

For the aLEFT, that we will construct in Sec. 7.4, an analysis of the shift-symmetric limit can be performed in a similar fashion as the one presented here. Therefore, we will skip the discussion of the shift symmetric limit there.

7.3.4 CP Violation in the aSMEFT

Adding C and P transformations to the Hilbert series as described in Section 2.5.2 enables us to count the number of CP-odd and CP-even parameters in the effective Lagrangian separately. In Tab. 7.1 we have summarised the results for the aSMEFT with and without a shift symmetry for the ALP. Furthermore, we show the number of CP-violating couplings which are the number of CP-odd couplings that cannot be removed after using the freedom of performing rephasing transformations on all fermion fields that leave the renormalisable

Dim.	$\text{aSMEFT}_{\text{PQ}}$			$\text{aSMEFT}_{\not{\text{PQ}}}$		
	CP-even	CP-odd	CP-violating	CP-even	CP-odd	CP-violating
5	6	0	0	6	9	9
	29	15	9	30	33	27
6	1	0	0	11	7	6
	1	0	0	40	36	24
7	26	18	18	60	86	81
	189	167	128	1647	1830	1062
8	22	10	6	123	85	61
	271	249	33	2872	2667	912
9	427	356	332	942	1042	945
	12662	12336	6807	37345	37999	20476
10	356	289	134	1678	1511	979
	12702	12299	1733	95929	94872	21555
11	7053	6717	5926	15978	16437	13942
	513504	509377	235519	1651318	1654805	702019
12	7491	7184	2812	29909	29143	16295
	910536	908691	60630	4301474	4296142	759162
13	127404	125817	104553	285800	287958	227861
	19442371	19421423	7978922	61499879	61539007	22689934
14	166364	164745	54104	583011	579234	279807
	45535198	45521724	2494107	194761001	194708399	25144913
15	2400015	2392287	1868885	5279487	5289614	3909730
	810986291	810842733	284971909	2403111000	2403360999	764583481

Table 7.1: Number of CP-even, CP-odd and CP-violating operators for $\text{aSMEFT}_{\text{PQ}}$ (left) and $\text{aSMEFT}_{\not{\text{PQ}}}$ (right) from dimension 5 to 15. In each dimension, the two rows correspond to $N_f = 1$ and $N_f = 3$ respectively.

part of the Lagrangian invariant, i.e. $U(1)^3_{L_i} \times U(1)_B$ rephasings for the aSMEFT. In this analysis we turn on one operator at a time, such that all possible rephasings can be used for each operator.

In the bosonic sector this counting is straightforward, because all bosonic operators in our basis are eigenstates of CP. Then, those operators which transform with a sign under CP are CP-violating. In the fermionic sector the identification of all CP-violating couplings is complicated by flavour transformations, which can be performed on top of the CP transformation to remove CP-violating parameters. Therefore, it is advisable to use flavour invariants to characterise CP-violating parameters as was discussed for the SM in Sec. 2.1.2 and for the SMEFT in Sec. 2.2.3. The flavour invariants automatically keep track of this additional reparameterisation freedom that we have just described.

In the aSMEFT$_{\not{PQ}}$, the dimension-5 CP-violating Hilbert series is given by[9]

$$\mathcal{H}^{\not{PQ}}_{5,\mathrm{CPV}} = a^5 + aB^2 + aW^2 + aG^2 + a^3H^2 + aH^4 + 3aLHe + 9aQHu + 9aQHd\,, \tag{7.26}$$

from which we can count the number of CP-violating parameters in each operator. In the fermion sector of the dimension-5 aSMEFT$_{\not{PQ}}$, all couplings are described by 3 generic complex 3×3 matrices C_{ae}, C_{au} and C_{ad}.

Following the procedure for the SMEFT operators [103, 104] summarised in Sec. 2.2.3, the following flavour invariants can be found capturing all primary sources of CP violation in the leptonic sector of the EFT[10]

$$\mathrm{Re}\,\mathrm{Tr}\left(C_{ae}Y_e^\dagger\right), \quad \mathrm{Re}\,\mathrm{Tr}\left(X_eC_{ae}Y_e^\dagger\right), \quad \mathrm{Re}\,\mathrm{Tr}\left(X_e^2C_{ae}Y_e^\dagger\right), \tag{7.27}$$

where we repeat the definition of $X_{u,d,e} = Y_{u,d,e}Y^\dagger_{u,d,e}$. Note, that the number of flavour invariants exactly match the corresponding term $+3aLHe$ in the Hilbert series. Setting these invariants to zero yields the sufficient and necessary conditions for CP conservation in the presence of the operator at hand. In the quark sector we find the following independent invariants

$$\begin{gathered} L_{0000}\left(C_{au}Y_u^\dagger\right),\ L_{1000}\left(C_{au}Y_u^\dagger\right),\ L_{0100}\left(C_{au}Y_u^\dagger\right),\ L_{1100}\left(C_{au}Y_u^\dagger\right),\ L_{0110}\left(C_{au}Y_u^\dagger\right), \\ L_{2200}\left(C_{au}Y_u^\dagger\right),\ L_{0220}\left(C_{au}Y_u^\dagger\right),\ L_{1220}\left(C_{au}Y_u^\dagger\right),\ L_{0122}\left(C_{au}Y_u^\dagger\right), \end{gathered} \tag{7.28}$$

where we have defined $L_{abcd}(C) = \mathrm{Re}\,\mathrm{Tr}\left(X_u^aX_d^bX_u^cX_d^dC\right)$ and similar relations hold true in the down sector with $C_{au}Y_u^\dagger \to C_{ad}Y_d^\dagger$. These are exactly the flavour invariants, we have already found in the previous chapter in Eq. (6.48). Here, we have verified this counting by comparing the 18 flavour invariants to the terms $+9aQHu + 9aQHd$ in the Hilbert series. In total, 21 CP-odd flavour invariants for $N_f = 3$ have to vanish for CP conservation in the fermionic sector of the EFT and 6 CP-odd operators in the bosonic sector have to be set to zero, which can be easily identified in Tab. 7.7. This is consistent with the counting in Tab. 7.1. For higher dimensional operators, the CP-even, CP-odd and CP-violating Hilbert series can be found in Ref. [2].

In the dimension-5 aSMEFT$_{\mathrm{PQ}}$, all couplings are described by 5 hermitian matrices in the derivatively coupled basis. Interestingly, no primary sources of CP violation can be written down for the leptonic sector because there exist no quantities charged under rephasings of the lepton fields in the SM Lagrangian. This is consistent with the results in the aSMEFT$_{\not{PQ}}$ where we have to impose shift symmetry on the invariants in Eq. (7.27). Because these CP invariants are identical to those capturing the shift symmetry presented in Eq. (6.22), there

[9] We have redefined $\check{\phi}$ to ϕ to simplify the notation here.

[10] As introduced in Sec. 2.2.3, we denote all CP-odd couplings as primary, which can form a flavour-invariant quantity at leading order in the EFT. For instance, the complex 3×3 matrix C_{ae} has 9 CP-odd parameters. However, there only exist three flavour-invariant CP-odd quantities at the leading order in the EFT expansion as can be seen in Eq. (7.27). All other CP-odd parameters can only appear at subleading orders in the EFT expansion. This changes in the quark sector due to the existence of the CKM matrix which being charged under rephasings can give rise to more primary sources of CP violation. See also Ref. [103].

are no remaining primary sources of CP violation in the leptonic sector of the shift-symmetric EFT. This is also captured by the CP-violating Hilbert series

$$\mathcal{H}_{5,\mathrm{CPV}}^{\mathrm{PQ}} = 3\partial a\, Q^2 + 3\partial a\, u^2 + 3\partial a\, d^2\,, \tag{7.29}$$

where no terms including lepton fields are present due to the application of lepton family number rephasings.

In the quark sector we find the following CP-violating invariants for the couplings $C_{\partial aQ}$

$$\tilde{L}_{1100}\left(C_{\partial aQ}\right),\ \tilde{L}_{2200}\left(C_{\partial aQ}\right),\ \tilde{L}_{1122}\left(C_{\partial aQ}\right), \tag{7.30}$$

where $\tilde{L}_{abcd}(C) = \mathrm{Im}\,\mathrm{Tr}\left(X_u^a X_d^b X_u^c X_d^d C\right)$[11] and similar relations can be found for $C_{\partial au}$ and $C_{\partial ad}$ by replacing $C_{\partial aQ} \to Y_u C_{\partial au} Y_u^\dagger$ and $C_{\partial aQ} \to Y_d C_{\partial ad} Y_d^\dagger$ respectively. The number of flavour invariants matches precisely the number of CP-violating couplings counted by the Hilbert series in Eq. (7.29).

We can again compare with the EFT of a generic pseudoscalar by taking the shift-symmetric limit. For the ALP-Yukawa couplings in the aSMEFT$_{\not{PQ}}$, we have found 18 flavour-invariant quantities at leading order. Following our discussion in Chap. 6, 9 of those have to be set to zero, in order to obtain a shift-symmetric Lagrangian giving agreement with the shift-symmetric theory in the Yukawa basis. We can furthermore compare with the counting in Tab. 7.1. In the aSMEFT$_{\mathrm{PQ}}$, all CP-violating couplings are forbidden in the bosonic sector and, as we just counted, there are 9 CP-odd flavour invariants for $N_f = 3$. This is consistent with the counting at dimension-5 in Tab. 7.1.

7.4 aLEFT

Following our previous implementation of the SM particle spectrum extended with an ALP for the Hilbert series, it is relatively easy to also construct the Hilbert series for the EFT below the electroweak scale.

As discussed in Section 7.2, the three main differences are the different particle content where the heavy particles of the SM, the W, Z, h and t, now have been integrated out, the fact that the left-handed fermions are no longer related through their appearance in $SU(2)$ doublets and the smaller gauge group $SU(3)_c \times U(1)_{\mathrm{em}}$ due to the breaking of the electroweak symmetry group $SU(2)_L \times U(1)_Y$. Since the gauge group below the EW scale is only $SU(3)_c \times U(1)_{\mathrm{em}}$, both a linear and a non-linear realisation of the EW symmetry can be captured in the LEFT. Hence, we can describe effects of HEFT-like ALP couplings to the SM particles [194, 202, 315] in the LEFT extended with an ALP.

Knowledge about the effective description of interactions at those energies is also of phenomenological importance for experiments operating at these scales. For instance, exotic meson decays give strong bounds on the flavourful couplings of the ALP to the SM fermions [189]. Running further to lower energies, constructing the QCD chiral Lagrangian [145,

[11] The difference between L and $\tilde{L}$ is the imaginary and real part that is taken for the respective invariants, such that both invariants capture the CP-violating couplings in the EFT.

[175, 212, 316] extended with an ALP and matching it to the aLEFT would complete a full EFT description beyond leading order at all scales. Here, depending on the mass of the axion, it can also be integrated out above the QCD scale and captured in a low energy EFT of the QCD mesons without the ALP in the particle spectrum.

7.4.1 $\mathbf{aLEFT_{PQ}}$

We compute the Hilbert series for the effective operators order by order in the same way as for the EFT above the electroweak scale. Up to mass dimension 7, we find

$$\begin{aligned}
\mathcal{H}_5^{\mathrm{aLEFT_{PQ}}} &= \partial a\, u_L u_L^\dagger + \partial a\, u_R u_R^\dagger + \partial a\, d_L d_L^\dagger + \partial a\, d_R d_R^\dagger + \partial a\, \nu_L \nu_L^\dagger + \partial a\, e_L e_L^\dagger + \partial a\, e_R e_R^\dagger \\
&\quad - \partial a\, F_L \mathcal{D} - \partial a\, F_R \mathcal{D} - \partial a\, \mathcal{D}^3 \,, \\
\mathcal{H}_6^{\mathrm{aLEFT_{PQ}}} &= 0 \,, \\
\mathcal{H}_7^{\mathrm{aLEFT_{PQ}}} &= (\partial a)^2 u_L u_R + (\partial a)^2 u_L^\dagger u_R^\dagger + (\partial a)^2 d_L d_R + (\partial a)^2 d_L^\dagger d_R^\dagger + (\partial a)^2 \nu_L^2 + (\partial a)^2 \nu_L^{\dagger 2} \\
&\quad + (\partial a)^2 e_L e_R + (\partial a)^2 e_L^\dagger e_R^\dagger + \partial a\, u_L u_L^\dagger F_L + \partial a\, u_L u_L^\dagger F_R + \partial a\, u_L u_L^\dagger G_L \\
&\quad + \partial a\, u_L u_L^\dagger G_R + \partial a\, u_R u_R^\dagger F_L + \partial a\, u_R u_R^\dagger F_R + \partial a\, u_R u_R^\dagger G_L + \partial a\, u_R u_R^\dagger G_R \\
&\quad + \partial a\, d_L d_L^\dagger F_L + \partial a\, d_R d_R^\dagger F_L + \partial a\, d_L d_L^\dagger F_R + \partial a\, d_R d_R^\dagger F_R + \partial a\, d_L d_L^\dagger G_L \\
&\quad + \partial a\, d_R d_R^\dagger G_L + \partial a\, d_L d_L^\dagger G_R + \partial a\, d_R d_R^\dagger G_R + \partial a\, \nu_L \nu_L^\dagger F_L + \partial a\, \nu_L \nu_L^\dagger F_R \\
&\quad + \partial a\, e_L e_L^\dagger F_L + \partial a\, e_R e_R^\dagger F_L + \partial a\, e_L e_L^\dagger F_R + \partial a\, e_R e_R^\dagger F_R \,,
\end{aligned} \tag{7.31}$$

and more results can be found in Ref. [2]. With these numbers as a guide, the effective operators can be constructed, which like in the aSMEFT is mostly straightforward up to some relations among operators due to relations in the algebra of the groups appearing in the problem. Due to the increased number of independent fermions below the electroweak scale, one particularly challenging class of operators to construct is those of 4-fermion operators coupled to ∂a at dimension 8. Here, one has to keep track of all the Fierz identities among the operators (see e.g. Refs. [272, 317]), which eventually leads to our set of non-redundant operators found in Tab. 7.10.

Below the EW scale, the exact flavour symmetries of the renormalisable Lagrangian change with respect to those above the EW scale, as the left-handed fermions no longer come together in doublets. Therefore, all mass terms can be diagonalised and the misalignment captured by the CKM matrix that one finds above the EW scale is only present at $1/m_W^2$ in the EFT expansion allowing for more possible rephasings for the quarks. As in the lepton sector above the EW scale, every quark flavour can now be rephased by itself instead of the universal baryon number rephasing. In the lepton sector, the charged leptons keep their lepton family number rephasing properties while the neutrinos do not benefit from any flavour symmetries due to the lepton number breaking mass term $\bar{\nu}_L \nu_L^c$ + h.c. that we allow for in the most generic low-energy Lagrangian. These classically conserved symmetries lead to $N_u + N_d + N_e$ conserved currents that can be used in the dimension-5 Lagrangians to remove operators by imposing $\partial_\mu j^\mu = 0$ after integrating by parts. As in the aSMEFT, we have to impose these conditions by hand after calculating the Hilbert series. Furthermore, we have to add the anomalous

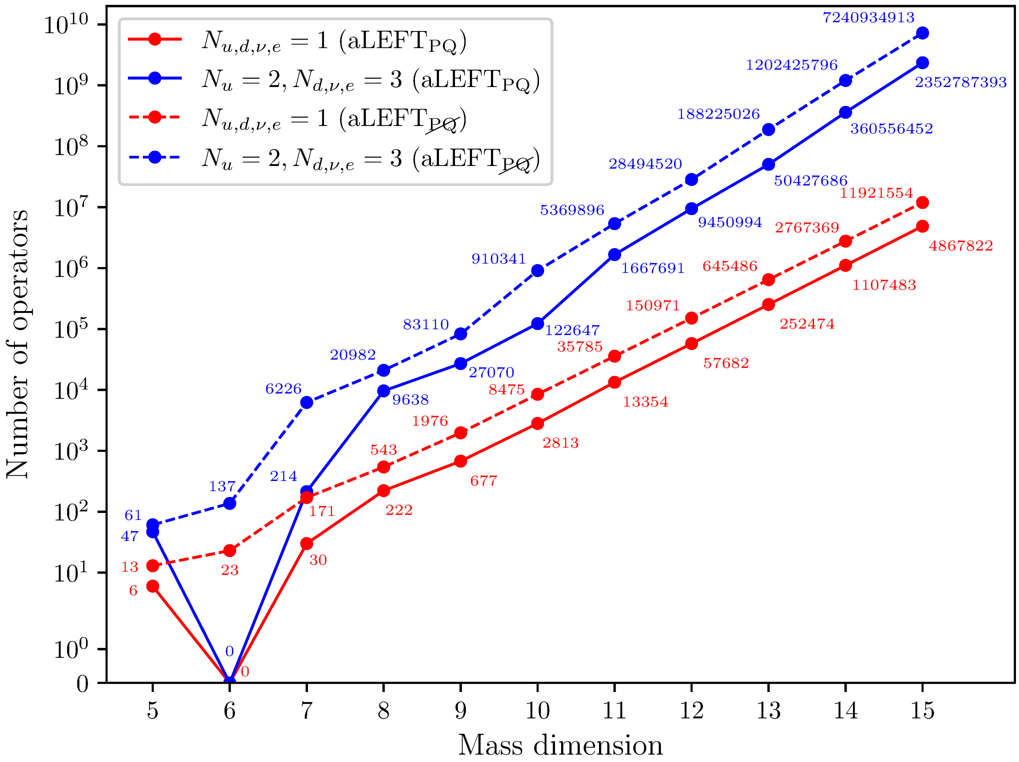


Figure 7.2: The number of operators in the aLEFT with and without a shift symmetry for the ALP plotted against the mass dimension for $N_u = N_d = N_\nu = N_e = 1$ and $N_u = 2, N_d = N_\nu = N_e = 3$ number of flavours. Note that the y-axis has a linear scaling between 0 and 1 to accommodate for the 0 at mass dimension 6.

operators $aF\widetilde{F}, aG\widetilde{G}$ to the operator basis by hand as well.

Our complete basis up to mass dimension 8 for an ALP coupled derivatively to all particles in the SM below the EW scale can be found in Tabs. 7.8, 7.9 and 7.10 in App. 7.B.1. The operator basis at mass dimension 5 in the aLEFT is consistent with the operators used in Ref. [212]. As before, we can use the ALP-independent terms in the Hilbert series as a sanity check for our implementation of the Hilbert series and compare them with the known results for the operator bases up to dimension 8 in the LEFT [291, 318, 319].

After computing the Hilbert series, we will repeat the analysis of the flavour dependence as was done for the aSMEFT. As before, we count the number of independent operators for a generic number of flavours using lepton and baryon number rephasings to single out the lepton and baryon number breaking operators. Using $N_\nu = N_e = N_d$[12] to keep the expressions

[12] We keep N_u independent here, since we want to take the limit $N_\nu = N_e = N_d = 3$, $N_u = 2$ later amounting to the usual flavour content of the EFT right below the EW scale after only the top quark out of all quarks is integrated out.

more concise, we find

$$
\begin{aligned}
\#\,\mathcal{O}_5^{\mathrm{aLEFT_{PQ}}} &= 2 - 2N_d + 5N_d^2 - N_u + 2N_u^2\,,\\
\#\,\mathcal{O}_6^{\mathrm{aLEFT_{PQ}}} &= 0\,,\\
\#\,\mathcal{O}_7^{\mathrm{aLEFT_{PQ}}} &= \left(18N_d^2 + 10N_u^2\right) + \left(N_d + N_d^2\right)\epsilon_L^2\,,\\
\#\,\mathcal{O}_8^{\mathrm{aLEFT_{PQ}}} &= \left(7 + 23N_d^2 + 36N_d^4 + 16N_d^3N_u + 14N_u^2 + 52N_d^2N_u^2 + 8N_u^4\right)\\
&\quad + \left(-\frac{4N_d^2}{3} + \frac{16N_d^4}{3} + 16N_d^3N_u + 16N_d^2N_u^2\right)\epsilon_B\epsilon_L\\
&\quad + \left(-N_d + \frac{7N_d^2}{3} + \frac{26N_d^4}{3} + 16N_d^3N_u + 4N_d^2N_u^2\right)\epsilon_L^2\,.
\end{aligned}
\tag{7.32}
$$

As before, shift symmetry protects from lepton number breaking due to the specific structure of the derivatively coupled ALP. The lepton number-breaking, gauge-invariant neutrino mass term $\bar{\nu}_L^c\nu_L + \mathrm{h.c.}$ that can be written down below the EW scale allows for lepton number breaking already at dimension 7 w.r.t the lepton number-breaking terms at dimension 8 in the EFT above the EW scale.

7.4.2 aLEFT$_{\not{\text{PQ}}}$

We will now proceed by calculating the Hilbert series for the LEFT extended with a generic scalar field a that can but no longer necessarily has to be connected to the spontaneous breaking of a PQ symmetry. The first two orders in the expansion of the Hilbert series in the mass dimension of the operators are given by

$$
\begin{aligned}
\mathcal{H}_5^{\mathrm{aLEFT_{\not{PQ}}}} &= a^5 + a^2u_Lu_R + a^2u_L^\dagger u_R^\dagger + a^2d_Ld_R + a^2d_L^\dagger d_R^\dagger + a^2\nu_L^2 + a^2\nu_L^{\dagger 2} + a^2e_Le_R\\
&\quad + a^2e_L^\dagger e_R^\dagger + aF_L^2 + aF_R^2 + aG_L^2 + aG_R^2\,,\\
\mathcal{H}_6^{\mathrm{aLEFT_{\not{PQ}}}} &= a^6 + a^3u_Lu_R + a^3u_L^\dagger u_R^\dagger + a^3d_Ld_R + a^3d_L^\dagger d_R^\dagger + a^3\nu_L^2 + a^3\nu_L^{\dagger 2} + a^3e_Le_R\\
&\quad + a^3e_L^\dagger e_R^\dagger + a^2F_L^2 + a^2F_R^2 + a^2G_L^2 + a^2G_R^2 + au_Lu_RF_L + au_Lu_RG_L\\
&\quad + au_L^\dagger u_R^\dagger F_R + au_L^\dagger u_R^\dagger G_R + ad_Ld_RF_L + ad_L^\dagger d_R^\dagger F_R + ad_Ld_RG_L\\
&\quad + ad_L^\dagger d_R^\dagger G_R + ae_Le_RF_L + ae_L^\dagger e_R^\dagger F_R\,.
\end{aligned}
\tag{7.33}
$$

From these two orders it is already clear that the Hilbert series features the same structure as the Hilbert series of the aSMEFT. As before, operators can simply be built by multiplying operators at the previous mass dimension with a due to the singlet pseudo-scalar nature of the ALP. Furthermore, we have checked up to mass dimension 15, that there exists a similar PQ-breaking isolation condition beyond dimension 5 that we have found for the aSMEFT

$$
\mathcal{H}_n^{\mathrm{aLEFT_{\not{PQ}}}} = a\,\mathcal{H}_{n-1}^{\mathrm{aLEFT_{\not{PQ}}}} + a\,\mathcal{H}_{n-1}^{\mathrm{LEFT}} + \mathcal{H}_n^{\mathrm{aLEFT_{PQ}}}\left(\partial a \to a\mathcal{D}\right)
\tag{7.34}
$$

Therefore the same discussion about shift symmetry that we will present in the following section also applies to the aLEFT. The complete operator basis at dimension 5 can be found in

Tab. 7.13. Based on the shift-breaking isolation condition in Eq. (7.34), the higher dimensional operator bases can be constructed easily, see App. 7.B.2 for details.

In the aLEFT, one finds that the operators coupling one ALP field to the fermions naively already appear at dimension 4 by studying the renormalisable part of the Lagrangian

$$\begin{aligned}\mathcal{L}^a_{\leq 4} =& \frac{1}{2}\partial_\mu a \partial^\mu a - \frac{m^2_{a,0}}{2}a^2 + C_{a^3}a^3 + C_{a^4}a^4 + \frac{a}{f}\left(\bar{u}_L C^{SR}_{au} u_R + \bar{d}_L C^{SR}_{ad} d_R + \bar{e}_L C^{SR}_{ae} e_R \right.\\ &\left. + \bar{\nu}_L C^{SR}_{a\nu} \nu^c_L + \text{h.c.}\right) ,\end{aligned} \tag{7.35}$$

that we have neglected up to this point. If one performs a matching of the aSMEFT to the aLEFT one obtains

$$\{C^{SR}_{au}, C^{SR}_{ad}, C^{SR}_{ae}\} = \frac{v}{\sqrt{2}}\{C_{au}, C_{ad}, C_{ae}\} \quad \text{and} \quad C^{SR}_{a\nu} = \frac{v^2}{2}C_{aLH} \tag{7.36}$$

after expanding the Higgs around its VEV v and the operators can be identified with dimension-5 and dimension-6 operators in the aSMEFT. This leads to subtleties in the counting of the operators, since the dimension-4 couplings are not properly counted by the Hilbert series and we have to rely on the next mass dimension to perform a comparison to the derivative basis.

We perform this comparison by considering the numbers in Fig. 7.2 to see if we can understand the results in terms of the invariants constructed in the low-energy limit in Chap. 6. As in the dimension-5 aSMEFT, the derivatively coupled ALP interactions with the fermions become redundant in the presence of the dimension-5 ALP Yukawa couplings for a generic pseudoscalar. We have just discussed that the Yukawa ALP operators already appear at mass dimension 4 in the aLEFT, which we have to keep in mind in our discussion. Looking at Tab. 7.13, we can see that the same number of ALP-fermion interactions appear at dimension 4 and dimension 5 in the aLEFT because one operator can just be obtained by multiplying the other one by a. Hence, we can rely on the numbers at dimension 5 to understand the counting.

The difference at dimension 5 in Fig. 7.2 can be explained as follows. Following our discussion in Sec. 6.3.3, the 13 conditions for shift invariance reduce to 8 invariants below the electroweak scale at the leading order in the EFT. The four invariants appearing due to the correlations induced by the left-handed quark doublet get shifted to higher mass dimensions in the $1/m^2_W$ expansion after breaking the EW symmetry in the aSMEFT[13] and one more invariant is removed because the top quark is integrated out. With respect to the discussion in Chap. 6, where we neglected neutrino masses, we also allow for lepton number-breaking neutrino masses here. This implies that there are an additional 3 relations in the fermionic sector, totalling 11 conditions that have to be imposed in the fermionic sector of the EFT below the EW scale for shift invariance to be preserved. Then, we have to subtract the 11 conditions obtained from the fermionic sector at dimension 4 (which are counted in the same way at dimension 5), the 1 condition obtained from removing the operator a^5 and the 2 conditions obtained from removing aFF and aGG from the 61 terms at dimension 5 which yields exactly the 47 terms in Fig. 7.2.

[13] If one starts from a HEFT-like scenario, these correlations will not be there in the first place which is both captured in the aLEFT in higher-dimensional operators upon matching to a HEFT-/SMEFT-like scenario.

We have also once more performed the counting of operators for each mass dimension by setting all spurions to unity and applying the same procedure as before to single out the lepton and baryon number violating terms. We find

$$\begin{aligned}
\#\,\mathcal{O}_5^{\mathrm{aLEFT}_{\not P \not Q}} &= \left(5 + 4N_d^2 + 2N_u^2\right) + \left(N_d + N_d^2\right)\epsilon_L^2\,,\\
\#\,\mathcal{O}_6^{\mathrm{aLEFT}_{\not P \not Q}} &= \left(5 + 10N_d^2 + 6N_u^2\right) + 2N_d^2\epsilon_L^2\,,\\
\#\,\mathcal{O}_7^{\mathrm{aLEFT}_{\not P \not Q}} &= \left(7 + \frac{131N_d^2}{4} + \frac{3N_d^3}{2} + \frac{87N_d^4}{4} + 10N_d^3N_u + 19N_u^2 + 32N_d^2N_u^2 + 5N_u^4\right)\\
&\quad + \left(-\frac{4N_d^2}{3} - 2N_d^3 + \frac{10N_d^4}{3} - 4N_d^2N_u + 10N_d^3N_u + 10N_d^2N_u^2\right)\epsilon_B\epsilon_L\\
&\quad + \left(N_d + 3N_d^2 + 2N_d^3 + 6N_d^4 + 10N_d^3N_u + N_dN_u^2 + 3N_d^2N_u^2\right)\epsilon_L^2\\
&\quad + \left(-\frac{N_d^2}{6} + \frac{N_d^4}{6}\right)\epsilon_L^4\,, \qquad (7.37)\\
\#\,\mathcal{O}_8^{\mathrm{aLEFT}_{\not P \not Q}} &= \left(14 + \frac{335N_d^2}{4} - \frac{N_d^3}{2} + \frac{303N_d^4}{4} + 34N_d^3N_u + 53N_u^2 + 110N_d^2N_u^2 + 17N_u^4\right)\\
&\quad + \left(-\frac{4N_d^2}{3} + 2N_d^3 + \frac{34N_d^4}{3} + 4N_d^2N_u + 34N_d^3N_u + 34N_d^2N_u^2\right)\epsilon_B\epsilon_L\\
&\quad + \left(4N_d + 10N_d^2 - 3N_d^3 + 19N_d^4 + 34N_d^3N_u - N_dN_u^2 + 9N_d^2N_u^2\right)\epsilon_L^2\\
&\quad + \left(-\frac{N_d^2}{6} + \frac{N_d^4}{6}\right)\epsilon_L^4\,.
\end{aligned}$$

Again, we only show the leading results here and the remaining results with full spurion and flavour dependence can be found in Ref. [2]. Note, that due to the operator $a\bar{\nu}\nu_L^c + \text{h.c.}$, a lepton-number violating term can already be written down at dimension 4 (it has the same dependence on the number of flavours as the corresponding term at mass dimension 5 quoted at the end of $\#\,\mathcal{O}_5^{\mathrm{aLEFT}_{\not P \not Q}}$ in Eq. (7.37)), which is the operator that captures the effects of the derivatively coupled operator $\partial_\mu a\,\bar{\nu}_L\gamma^\mu\nu_L$ that does not violate lepton number. This only makes sense if the coefficient of $a\bar{\nu}\nu_L^c + \text{h.c.}$ is proportional to the renormalisable spurion of lepton number breaking m_ν which is indeed the case as one can check from the usual relations (c.f. Eq. (2.78)) expected at dimension 5.

7.4.3 CP Violation in the aLEFT

In this section we will discuss CP transformations in the aLEFT. The same general discussion as for the aSMEFT in Section 7.3.4 applies. As discussed before, in the aLEFT all fermions are independent fields and are no longer subject to correlations through linear electroweak symmetry breaking. This yields the larger exact flavour group $U(1)^3_{e_i}\times U(1)^2_{u_i}\times U(1)^3_{d_i}$, leaving the renormalisable SM Lagrangian below the EW scale invariant. Keeping this in mind, we find the following Hilbert series counting the CP-violating couplings in the $\mathrm{aLEFT}_{\not P \not Q}$ at dimension 5

$$\mathcal{H}_{5,\mathrm{CPV}}^{\mathrm{aLEFT}_{\not P \not Q}} = a^5 + aF^2 + aG^2 + 3a^2e_Le_R + 6a^2\nu_L^2 + 2a^2u_Lu_R + 3a^2d_Ld_R\,, \qquad (7.38)$$

Dim.	aLEFT_{PQ}			$\text{aLEFT}_{\cancel{\text{PQ}}}$		
	CP-even	CP-odd	CP-violating	CP-even	CP-odd	CP-violating
5	6 30	0 17	0 3	6 30	7 31	7 17
6	0 0	0 0	0 0	12 69	11 68	11 32
7	15 107	15 107	15 49	68 2995	103 3231	85 634
8	116 4830	106 4808	72 698	294 10620	249 10362	173 1467
9	370 13691	307 13379	205 1860	951 41320	1025 41790	709 6120
10	1444 61565	1369 61082	901 8224	4312 455647	4163 454694	2521 33450
11	6836 836128	6518 831563	3759 53634	17727 2683815	18058 2686081	10168 163719
12	28965 4726245	28717 4724749	15483 271917	75775 14249141	75196 14245379	38924 763605
13	126851 25222133	125623 25205553	63572 1305402	321876 94093443	323610 94131583	158051 3848880
14	554379 180283648	553104 180272804	262485 6861666	1385189 601237390	1382180 601188406	630296 19339749
15	2436838 1176447813	2430984 1176339580	1084823 35693696	5956959 3620363967	5964595 3620570946	2569894 98145863

Table 7.2: Number of CP-even, CP-odd and CP-violating operators for aLEFT_{PQ} (left) and $\text{aLEFT}_{\cancel{\text{PQ}}}$ (right) from dimension 5 to 15. In each dimension, the two rows correspond to $N_{u,d,e,\nu} = 1$ and $N_u = 2$, $N_{d,e,\nu} = 3$ respectively.

while the counting of CP-even, CP-odd and CP-violating couplings in the aLEFT up to mass dimension 15 can be found in Tab. 7.2.

The number of primary CP-odd invariants decreases in the quark sector and we find the following three invariants in the $\text{aLEFT}_{\cancel{\text{PQ}}}$ at dimension 4[14]

$$\mathrm{Re}\,\mathrm{Tr}\left(C_{af}^{SR} m_f^\dagger\right), \quad \mathrm{Re}\,\mathrm{Tr}\left(X_f C_{af}^{SR} m_f^\dagger\right), \quad \mathrm{Re}\,\mathrm{Tr}\left(X_f^2 C_{af}^{SR} m_f^\dagger\right) \tag{7.39}$$

for each type of fermion $f = u, d, e, \nu$. Here, $X_{u,d,e,\nu} = m_{u,d,e,\nu} m_{u,d,e,\nu}^\dagger$.

As we have discussed in the last section, the leading ALP-fermion interactions will move to dimension 4 in the aLEFT that can be matched to the dimension-5 interactions in the aSMEFT. We can still use the flavour invariants at dimension 4 to check the results for the dimension-5 ALP-Yukawa operators because they have the same structure in flavour space.

[14]If we set $N_u = 2$ and $N_{d,e,\nu} = 3$, there will be only two non-redundant flavour invariants for $f = u$, and in total $2 + 3 \times 3 = 11$ flavour invariants for fermions $f = u, d, e, \nu$.

We just have to keep track of the CP properties which is different for a and a^2 multiplying the fermion bilinear. However, since completely generic as well as symmetric coupling matrices have the same amount of CP-even and CP-odd parameters, the numbers do not change here.

The 11 CP-odd flavour invariants together with the 3 CP-odd bosonic operators at leading order give 14 CP-violating parameters that can appear in observables at the leading order in the EFT expansion. Comparing this to the expression of the CP-violating Hilbert series in Eq. (7.38), we find what looks like a mismatch between our counting with flavour invariants and the Hilbert series in the neutrino sector. However, one has to keep in mind that the Hilbert series counts all CP-violating couplings, i.e. all couplings that are CP-odd and cannot possibly be removed by rephasings of the fermion fields. The flavour invariants capture all physical degrees of freedom that can interfere with the SM at leading order. These numbers agree if there is a CP-odd rephasing invariant of the Wilson coefficient corresponding to the flavour invariant at the same order in the EFT power counting.

The Wilson coefficients of the electrons, for instance, allows for the CP-odd rephasing invariants $C_{ae,ii}$ at leading order in the EFT corresponding to the flavour invariants $\mathrm{Re}\,\mathrm{Tr}\Big(X_e^{0,1,2} C_{ae}^{SR} m_e^\dagger\Big)$ that capture the interference of the EFT and the SM. Due to the Majorana nature of the neutrinos, no rephasing invariant exists at leading order in the EFT that only contains the Wilson coefficient of the effective ALP-neutrino operator. Only after using the spurious transformation of the neutrino mass term under rephasings of the neutrino fields, one can build a rephasing invariant quantity which are exactly the flavour invariants shown in Eq. (7.39). This is not captured by the Hilbert series, as it only counts the number of parameters for each effective operator which cannot possibly be removed by a rephasing. Once the difference between the number of CP-violating parameters (6) and those parameters that can interfere with the SM (3) is taken into account, the numbers in Tab. 7.2 and the counting using the flavour invariants matches again. For operators at higher mass dimensions, similar consideration should be taken for operators involving neutrinos.

Turning to the $\mathrm{aLEFT}_{\mathrm{PQ}}$, we find

$$\mathcal{H}_{5,\mathrm{CPV}}^{\mathrm{aLEFT}_{\mathrm{PQ}}} = 3\partial a\, \nu_L^2\,. \tag{7.40}$$

All CP-odd bosonic operators are forbidden by the shift symmetry. In the fermion sector all couplings are hermitian matrices whose phases can not interfere with the renormalisable part of the Lagrangian due to the lack of a parameter that is charged under rephasings below the electroweak scale. Therefore, from our flavour invariant analysis we expect no CP-violating parameters that can interfere with the renormalisable part of the Lagrangian. This is compatible with Eq. (7.40) if the neutrinos are properly taken into account as we just discussed for the $\mathrm{aLEFT}_{\not{\mathrm{PQ}}}$.

7.5 Application: Positivity Bounds in the ALP EFT

As an application of our basis, we can study the positivity bounds that are enforced by fundamental principles of Lorentz-invariant QFT: analyticity, causality and unitarity [320, 321]. The bounds can be imposed by using the optical theorem and contour integrals to relate elastic 2-to-2 amplitudes in the forward limit, reduced by the Mandelstam variable s^2, to cross-sections, which are fundamentally positive objects. Interpreting the low-energy as an EFT, the amplitudes can be computed in terms of the Wilson coefficient of the EFT. Due to the momentum behaviour of the amplitudes, computing the residue of $\mathcal{A}/s^2$ corresponds to differentiating the amplitude w.r.t. s^2. By imposing the minimal conditions of analyticity, causality and unitarity on the Lorentz-invariant UV theory and its EFT, the positivity bounds to be derived below have to hold.

The bounds for the operators in the ALP EFT have in the meantime appeared in Refs. [322, 323], while Ref. [2] and this thesis were written. We will briefly reproduce the results here, using `FeynArts` [324], `FeynRules` [325] and `FormCalc` [326] to compute the elastic forward amplitudes. Considering the 2-to-2 scattering of a superposition of the ALP a and any of the components of the Higgs fields $H = (\phi_1 + i\phi_2, \phi_3 + i\phi_4)$ gives the following generic structure of the amplitude

$$\mathcal{A}_{\phi\phi\to\phi\phi}(s,t) = \#\frac{C}{f^4}\left(s^2+t^2+u^2\right), \tag{7.41}$$

with some positive numerical prefactor # depending on which particles are scattered. In the forward limit $(t \to 0)$ this reduces to

$$\mathcal{A}_{\phi\phi\to\phi\phi}(s) = \mathcal{A}_{\phi\phi\to\phi\phi}(s, t\to 0) = 2\#\frac{C}{f^4}s^2 \tag{7.42}$$

by using $s+t+u=0$ ($s=-u$ in the forward limit) for massless particles in a 2-to-2 process. Scattering generic scalar states $s_1 s_2 \to s_1 s_2$ which are defined as

$$|s_1\rangle = \sum_{i=1}^{4} a_i|\phi_i\rangle + a_5|a\rangle\,, \qquad |s_2\rangle = \sum_{i=1}^{4} b_i|\phi_i\rangle + b_5|a\rangle \tag{7.43}$$

gives the following dependence in the forward limit

$$\begin{aligned}\mathcal{A}_{s_1s_2\to s_1s_2}(s) = s^2\Bigg[&4a_5^2b_5^2\frac{C_{\partial a4}}{f^4} + 2a_5b_5\left(a_1b_1+a_2b_2+a_3b_3+a_4b_4\right)\frac{C^{(1)}_{\partial a2DH2}}{f^4}\\ &+\frac{1}{2}\Big(a_5^2\left(b_1^2+b_2^2+b_3^2+b_4^2\right)+b_5^2\left(a_1^2+a_2^2+a_3^2+a_4^2\right)+2a_5b_5\left(a_1b_1+a_2b_2+a_3b_3+a_4b_4\right)\Big)\frac{C^{(2)}_{\partial a2DH2}}{f^4}\Bigg]\,.\end{aligned} \tag{7.44}$$

Making different choices for the a_i, b_i one can obtain different positivity bounds on the Wilson coefficients (see Ref. [322]). For instance, choosing $a_{1,\dots,4} = b_{1,\dots,4} = 0\,; a_5, b_5 = 1$ yields the positivity bound

$$C_{\partial a4} \geq 0 \tag{7.45}$$

on the operator only consisting of axion fields. Other choices can give positivity bounds on linear combinations of the Wilson coefficients appearing in Eq. (7.44).

We can get more bounds by considering amplitudes with fermions. In particular there are two elastic amplitudes which give non vanishing bounds, for both chiralities of fermions.

They generically have the following form in the forward limit

$$\begin{aligned}\mathcal{A}_{a\psi^+\to a\psi^+}(s) &= is\#\frac{C_{\partial a2\psi_L D}}{f^4}\langle 4|1|2] \,,\\ \mathcal{A}_{a\psi^-\to a\psi^-}(s) &= is\#\frac{C_{\partial a2\psi_R D}}{f^4}[4|1|2\rangle \,,\end{aligned} \tag{7.46}$$

where # is again some positive numerical factor which depends on the representation of the fermions under the SM gauge group. We can simplify the spinor structure following the discussion in Ref.s [327, 328]. We know that

$$\begin{aligned}-\langle 12\rangle [12] \langle 14\rangle [14] = -su &\overset{t\to 0}{=} s^2 \,,\\ \Longrightarrow [41]\langle 12\rangle &\overset{t\to 0}{\to} s \,.\end{aligned}$$

Therefore,

$$[4|1|2\rangle = [41]\langle 12\rangle \overset{t\to 0}{=} s \,. \tag{7.47}$$

Following the discussion in Ref. [329], we scatter superposition of flavour states. We get for the simplified amplitudes in the forward limit

$$u_{ip}u^*_{ir}\mathcal{A}_{a\psi^\pm_{ip}\to a\psi^\pm_{ir}}(s) = \#s^2 u_p u^*_r \frac{C_{\partial a2\psi_{R/L}D,pr}}{f^4} \,, \tag{7.48}$$

where we have trivially marginalised over the colour index i. Defining $\rho_{pr} = u_p u^*_r$ as in Ref. [329], we find the following bounds for the Wilson coefficients of the fermionic operators

$$C_{\partial a2\psi D,pr}\,\rho_{pr} \geq 0 \,. \tag{7.49}$$

Lastly, we can bound Wilson coefficients by considering amplitudes with vector bosons. In the forward limit the amplitudes have the following form

$$\mathcal{A}_{aV^+\to aV^+}(s) = -\#s^2\frac{C^{(2)}_{\partial a2V}}{f^4} \,, \tag{7.50}$$

where # is again a positive numerical prefactor. Then we get the following positivity bounds for the operators with vector bosons

$$C^{(2)}_{\partial a2V} \leq 0 \tag{7.51}$$

Note, that as for the fermion operators only the amplitude where the vectors have the same helicities is elastic. Therefore, only one kind of operator, $\mathcal{O}^{(2)}_{\partial a2V}$, out of the 3 operators with 2 ALPs and 2 field strengths at that mass dimension can contribute to the elastic amplitude in the forward limit.

Appendices to Chapter 7

7.A Operator Basis for the aSMEFT up to Mass Dimension 8

Using the Hilbert series as a guide, we have constructed independent operator bases for aSMEFT, encompassing dimensions up to 8, for both shift-symmetric and non-shift-symmetric theories, which are shown explicitly in the following two appendices.

7.A.1 With Shift Symmetry

For aSMEFT with a shift symmetry, the operator bases from dimension 5 to dimension 8 are constructed, they are grouped in Tabs. 7.3, 7.4, 7.5 and 7.6 respectively. To show the different classes of operators appearing in the operator basis we have defined a reduced Hilbert series, where we identify fermions with ψ, field strengths with X, and the Higgs with H, and also keeping ∂a as a building block. The Hilbert series with $N_f = 1$ for each mass dimension is reduced to the following

$$\begin{aligned}
\mathcal{H}_5^{\mathrm{PQ}} &= 5\partial a\,\psi^2 + 3aX^2\,, \qquad \mathcal{H}_6^{\mathrm{PQ}} = (\partial a)^2 H^2\,,\\
\mathcal{H}_7^{\mathrm{PQ}} &= 20\partial a\,\psi^2 X + 4\partial a\,X H^2\mathcal{D} + 7\partial a\,\psi^2 H^2 + \partial a\,H^4\mathcal{D} + 12\partial a\,\psi^2 H\mathcal{D}\,,\\
\mathcal{H}_8^{\mathrm{PQ}} &= (\partial a)^4 + 5(\partial a)^2\psi^2\mathcal{D} + 9(\partial a)^2 X^2 + 4\partial a\,\psi^4 + 2(\partial a)^2 H^2\mathcal{D}^2 + 4\partial a\,\psi^2 H^2\mathcal{D}\\
&\quad + (\partial a)^2 H^4 + 6(\partial a)^2\psi^2 H + \{2\partial a\,\psi^4\}\,,
\end{aligned} \tag{7.52}$$

where for the Hilbert series at dimension 5, we have taken care of the caveats discussed in Section 7.3.1, i.e., operator where the ALP is coupled to a Higgs current and the negative terms are removed, while we have added the aX^2 terms by hand. As already mentioned in Section 7.3.1, setting $N_f = 1$ will lead to vanishing terms. In order to construct an operator basis for general N_f, such vanishing terms should also be taken into account, which are given as additional terms in the brackets in Eq. (7.52) and the corresponding operators are marked with ($\star$) in the tables of operator bases. For instance, the additional terms $\{2\partial a\,\psi^4\}$ correspond to the operator $\mathcal{O}_{\partial aed}$ + h.c. in Tab. 7.6.

$\partial a\,\psi^2$		aX^2	
$\mathcal{O}_{\partial aL}$	$\partial_\mu a\left(\bar{L}\gamma^\mu L\right)$	$\mathcal{O}_{a\tilde{B}}$	$aB_{\mu\nu}\widetilde{B}^{\mu\nu}$
$\mathcal{O}_{\partial ae}$	$\partial_\mu a\left(\bar{e}\gamma^\mu e\right)$	$\mathcal{O}_{a\tilde{W}}$	$aW^I_{\mu\nu}\widetilde{W}^{I,\mu\nu}$
$\mathcal{O}_{\partial aQ}$	$\partial_\mu a\left(\bar{Q}\gamma^\mu Q\right)$	$\mathcal{O}_{a\tilde{G}}$	$aG^a_{\mu\nu}\widetilde{G}^{a,\mu\nu}$
$\mathcal{O}_{\partial au}$	$\partial_\mu a\left(\bar{u}\gamma^\mu u\right)$		
$\mathcal{O}_{\partial ad}$	$\partial_\mu a\left(\bar{d}\gamma^\mu d\right)$		

Table 7.3: Operators in the aSMEFT at mass dimension 5 with ∂a as a building block. Note that $\mathcal{O}_{\partial aH} = \partial^\mu a\left(H^\dagger i\overleftrightarrow{D}_\mu H\right)$ is a redundant operator and can be removed via a global hypercharge transformation [175, 212]. Imposing lepton and baryon number conservation at the level of the renormalisable Lagrangian, 3 (1) flavour-diagonal entries of the operators coupling the ALP to leptons (quarks), for instance $\mathcal{O}_{\partial aL,ii}$ and $\mathcal{O}_{\partial aQ,11}$, can be removed [176]. Furthermore, we have used that the shift in the operators of class aX^2 can be removed using anomalous chiral transformations on the fermion fields making the operators shift-symmetric without an explicit derivative on the axion field.

$(\partial a)^2 H^2$	
$\mathcal{O}_{\partial a^2 H^2}$	$\partial_\mu a\,\partial^\mu a\,\lvert H\rvert^2$

Table 7.4: Operators in the aSMEFT at mass dimension 6 with ∂a as a building block.

$\partial a\, \psi^2 X$		$\partial a\, X H^2 D$	
$\mathcal{O}_{\partial aLB}$	$\partial^\mu a\, \left(\bar{L}\gamma^\nu L\right) B_{\mu\nu}$	$\mathcal{O}_{\partial aHB}$	$\partial_\mu a \Big(H^\dagger i \overleftrightarrow{D}_\nu H\Big) B^{\mu\nu}$
$\mathcal{O}_{\partial aL\tilde{B}}$	$\partial^\mu a\, \left(\bar{L}\gamma^\nu L\right) \widetilde{B}_{\mu\nu}$	$\mathcal{O}_{\partial aH\tilde{B}}$	$\partial_\mu a \Big(H^\dagger i \overleftrightarrow{D}_\nu H\Big) \widetilde{B}^{\mu\nu}$
$\mathcal{O}_{\partial aeB}$	$\partial^\mu a\, \left(\bar{e}\gamma^\nu e\right) B_{\mu\nu}$	$\mathcal{O}_{\partial aHW}$	$\partial_\mu a \Big(H^\dagger i \overleftrightarrow{D}^I_\nu H\Big) W^{I,\mu\nu}$
$\mathcal{O}_{\partial ae\tilde{B}}$	$\partial^\mu a\, \left(\bar{e}\gamma^\nu e\right) \widetilde{B}_{\mu\nu}$	$\mathcal{O}_{\partial aH\tilde{W}}$	$\partial_\mu a \Big(H^\dagger i \overleftrightarrow{D}^I_\nu H\Big) \widetilde{W}^{I,\mu\nu}$
$\mathcal{O}_{\partial aQB}$	$\partial^\mu a\, \left(\bar{Q}\gamma^\nu Q\right) B_{\mu\nu}$	$\partial a\, \psi^2 H^2$	
$\mathcal{O}_{\partial aQ\tilde{B}}$	$\partial^\mu a\, \left(\bar{Q}\gamma^\nu Q\right) \widetilde{B}_{\mu\nu}$	$\mathcal{O}^{(1)}_{\partial aLH^2}$	$\partial_\mu a\, \left(\bar{L}\gamma^\mu L\right) \lvert H\rvert^2$
$\mathcal{O}_{\partial auB}$	$\partial^\mu a\, \left(\bar{u}\gamma^\nu u\right) B_{\mu\nu}$	$\mathcal{O}^{(2)}_{\partial aLH^2}$	$\partial_\mu a\, \left(\bar{L}\gamma^\mu \sigma^I L\right)\left(H^\dagger \sigma^I H\right)$
$\mathcal{O}_{\partial au\tilde{B}}$	$\partial^\mu a\, \left(\bar{u}\gamma^\nu u\right) \widetilde{B}_{\mu\nu}$	$\mathcal{O}_{\partial aeH^2}$	$\partial_\mu a\, \left(\bar{e}\gamma^\mu e\right) \lvert H\rvert^2$
$\mathcal{O}_{\partial adB}$	$\partial^\mu a\, \left(\bar{d}\gamma^\nu d\right) B_{\mu\nu}$	$\mathcal{O}^{(1)}_{\partial aQH^2}$	$\partial_\mu a\, \left(\bar{Q}\gamma^\mu Q\right) \lvert H\rvert^2$
$\mathcal{O}_{\partial ad\tilde{B}}$	$\partial^\mu a\, \left(\bar{d}\gamma^\nu d\right) \widetilde{B}_{\mu\nu}$	$\mathcal{O}^{(2)}_{\partial aQH^2}$	$\partial_\mu a\, \left(\bar{Q}\gamma^\mu \sigma^I Q\right)\left(H^\dagger \sigma^I H\right)$
$\mathcal{O}_{\partial aLW}$	$\partial^\mu a\, \left(\bar{L}\gamma^\nu \sigma^I L\right) W^I_{\mu\nu}$	$\mathcal{O}_{\partial auH^2}$	$\partial_\mu a\, \left(\bar{u}\gamma^\mu u\right) \lvert H\rvert^2$
$\mathcal{O}_{\partial aL\tilde{W}}$	$\partial^\mu a\, \left(\bar{L}\gamma^\nu \sigma^I L\right) \widetilde{W}^I_{\mu\nu}$	$\mathcal{O}_{\partial adH^2}$	$\partial_\mu a\, \left(\bar{d}\gamma^\mu d\right) \lvert H\rvert^2$
$\mathcal{O}_{\partial aQW}$	$\partial^\mu a\, \left(\bar{Q}\gamma^\nu \sigma^I Q\right) W^I_{\mu\nu}$	$\partial a\, \psi^2 H D + \text{h.c.}$	
$\mathcal{O}_{\partial aQ\tilde{W}}$	$\partial^\mu a\, \left(\bar{Q}\gamma^\nu \sigma^I Q\right) \widetilde{W}^I_{\mu\nu}$	$\mathcal{O}^{(1)}_{\partial aeHD}$	$\partial_\mu a \left(D^\mu \bar{L}\right) He$
$\mathcal{O}_{\partial aQG}$	$\partial^\mu a\, \left(\bar{Q}\gamma^\nu T^a Q\right) G^a_{\mu\nu}$	$\mathcal{O}^{(2)}_{\partial aeHD}$	$\partial_\mu a\, \bar{L} H \left(D^\mu e\right)$
$\mathcal{O}_{\partial aQ\tilde{G}}$	$\partial^\mu a\, \left(\bar{Q}\gamma^\nu T^a Q\right) \widetilde{G}^a_{\mu\nu}$	$\mathcal{O}^{(1)}_{\partial auHD}$	$\partial_\mu a \left(D^\mu \bar{Q}\right) \widetilde{H} u$
$\mathcal{O}_{\partial auG}$	$\partial^\mu a\, \left(\bar{u}\gamma^\nu T^a u\right) G^a_{\mu\nu}$	$\mathcal{O}^{(2)}_{\partial auHD}$	$\partial_\mu a\, \bar{Q} \widetilde{H} \left(D^\mu u\right)$
$\mathcal{O}_{\partial au\tilde{G}}$	$\partial^\mu a\, \left(\bar{u}\gamma^\nu T^a u\right) \widetilde{G}^a_{\mu\nu}$	$\mathcal{O}^{(1)}_{\partial adHD}$	$\partial_\mu a \left(D^\mu \bar{Q}\right) H d$
$\mathcal{O}_{\partial adG}$	$\partial^\mu a\, \left(\bar{d}\gamma^\nu T^a d\right) G^a_{\mu\nu}$	$\mathcal{O}^{(2)}_{\partial adHD}$	$\partial_\mu a\, \bar{Q} H \left(D^\mu d\right)$
$\mathcal{O}_{\partial ad\tilde{G}}$	$\partial^\mu a\, \left(\bar{d}\gamma^\nu T^a d\right) \widetilde{G}^a_{\mu\nu}$	$\partial a\, H^4 D$	
		$\mathcal{O}_{\partial aH^4}$	$\partial^\mu a \Big(H^\dagger i \overleftrightarrow{D}_\mu H\Big) \lvert H\rvert^2$

Table 7.5: Operators in the aSMEFT at mass dimension 7 with ∂a as a building block.

$(\partial a)^2 X^2$		$(\partial a)^2 \psi^2 D$	
$\mathcal{O}^{(1)}_{\partial a^2 B}$	$\partial_\mu a \partial^\mu a\, B_{\nu\rho} B^{\nu\rho}$	$\mathcal{O}_{\partial a^2 LD}$	$\partial_\mu a \partial_\nu a \left(\bar{L}\gamma^\mu \overleftrightarrow{D}^\nu L\right)$
$\mathcal{O}^{(2)}_{\partial a^2 B}$	$\partial_\mu a \partial^\nu a\, B^{\mu\rho} B_{\nu\rho}$	$\mathcal{O}_{\partial a^2 eD}$	$\partial_\mu a \partial_\nu a \left(\bar{e}\gamma^\mu \overleftrightarrow{D}^\nu e\right)$
$\mathcal{O}_{\partial a^2 \tilde{B}}$	$\partial_\mu a \partial^\mu a\, B_{\nu\rho} \widetilde{B}^{\nu\rho}$	$\mathcal{O}_{\partial a^2 QD}$	$\partial_\mu a \partial_\nu a \left(\bar{Q}\gamma^\mu \overleftrightarrow{D}^\nu Q\right)$
$\mathcal{O}^{(1)}_{\partial a^2 W}$	$\partial_\mu a \partial^\mu a\, W^I_{\nu\rho} W^{I,\nu\rho}$	$\mathcal{O}_{\partial a^2 uD}$	$\partial_\mu a \partial_\nu a \left(\bar{u}\gamma^\mu \overleftrightarrow{D}^\nu u\right)$
$\mathcal{O}^{(2)}_{\partial a^2 W}$	$\partial_\mu a \partial^\nu a\, W^{I,\mu\rho} W^I_{\nu\rho}$	$\mathcal{O}_{\partial a^2 dD}$	$\partial_\mu a \partial_\nu a \left(\bar{d}\gamma^\mu \overleftrightarrow{D}^\nu d\right)$
$\mathcal{O}^{(2)}_{\partial a^2 \tilde{W}}$	$\partial_\mu a \partial^\mu a\, W^I_{\nu\rho} \widetilde{W}^{I,\nu\rho}$	$(\partial a)^2 \psi^2 H + \text{h.c.}$	
$\mathcal{O}^{(1)}_{\partial a^2 G}$	$\partial_\mu a \partial^\mu a\, G^a_{\nu\rho} G^{a,\nu\rho}$	$\mathcal{O}_{\partial a^2 eH}$	$\partial_\mu a \partial^\mu a\, \bar{L} H e$
$\mathcal{O}^{(2)}_{\partial a^2 G}$	$\partial_\mu a \partial^\nu a\, G^{a,\mu\rho} G^a_{\nu\rho}$	$\mathcal{O}_{\partial a^2 uH}$	$\partial_\mu a \partial^\mu a\, \bar{Q} H u$
$\mathcal{O}_{\partial a^2 \tilde{G}}$	$\partial_\mu a \partial^\mu a\, G^a_{\nu\rho} \widetilde{G}^{a,\nu\rho}$	$\mathcal{O}_{\partial a^2 dH}$	$\partial_\mu a \partial^\mu a\, \bar{Q} H d$
$(\partial a)^4$		$(\partial a)^2 H^2 D^2$	
$\mathcal{O}_{\partial a^4}$	$\partial_\mu a \partial^\mu a \partial_\nu a \partial^\nu a$	$\mathcal{O}^{(1)}_{\partial a^2 DH^2}$	$\partial_\mu a \partial^\mu a D_\nu H^\dagger D^\nu H$
$(\partial a)^2 H^4$		$\mathcal{O}^{(2)}_{\partial a^2 DH^2}$	$\partial_\mu a \partial_\nu a D^\mu H^\dagger D^\nu H$
$\mathcal{O}_{\partial a^2 H^4}$	$\partial_\mu a \partial^\mu a \lvert H\rvert^4$		
$\not{B}$ and $\not{L}$ terms			
$\partial a\, \psi^4 + \text{h.c.}$		$\partial a\, \psi^2 H^2 D + \text{h.c.}$	
$\mathcal{O}_{\partial aLdu}$	$\partial_\mu a \left(\bar{L}^c L\right)\left(\bar{d}\gamma^\mu u\right)$	$\mathcal{O}^{(1)}_{\partial aLHD}$	$\partial_\mu a \left(\bar{L}^c H\right)\left(\tilde{H}^\dagger D^\mu L\right)$
$\mathcal{O}_{\partial aLQd}$	$\epsilon^{\alpha\beta\gamma} \partial_\mu a \left(\bar{L} d_\alpha\right)\left(\bar{Q}^c_\beta \gamma^\mu d_\gamma\right)$	$\mathcal{O}^{(2)}_{\partial aLHD}$	$\partial_\mu a \left(\bar{L}^c D^\mu H\right)\left(\tilde{H}^\dagger L\right)$
$\mathcal{O}_{\partial aed}$ $(\star)$	$\epsilon^{\alpha\beta\gamma} \partial_\mu a \left(\bar{d}^c_\alpha d_\beta\right)\left(\bar{e}\gamma^\mu d_\gamma\right)$		

Table 7.6: Operators in the aSMEFT at mass dimension 8 with ∂a as a building block. Note that the operator $\mathcal{O}_{\partial aed}$ marked with $(\star)$ only exists for $N_f \neq 1$ because otherwise all contractions of the antisymmetric colour structure will sum to zero (the first current in the operator is symmetric under $\alpha \leftrightarrow \beta$ for one generation of fermions).

7.A.2 Without Shift Symmetry

For aSMEFT without a shift symmetry, we can use the shift-breaking isolation condition in Eq. (7.20) to construct the operator basis.

$$\mathcal{L}_n^{\not{\text{PQ}}} = a\,\mathcal{L}_{n-1}^{\not{\text{PQ}}} + a\,\mathcal{L}_{n-1}^{\text{SMEFT}} + \mathcal{L}_n^{\text{PQ}} \tag{7.53}$$

for $n > 5$. We start with the dimension-5 operator basis shown in Tab. 7.7, the dimension-6, 7, and 8 operator bases can be constructed successively. For instance, the operators at dimension 6 can be constructed with $\mathcal{L}_6^{\not{\text{PQ}}} = a\,\mathcal{L}_5^{\not{\text{PQ}}} + a\,\mathcal{L}_5^{\text{SMEFT}} + \mathcal{L}_6^{\text{PQ}}$, where the operators in $\mathcal{L}_5^{\text{SMEFT}}$ have been shown in Ref. [63], and the dimension-6 shift-symmetric operator basis associated with $\mathcal{L}_6^{\text{PQ}}$ is given in Tab. 7.4. The construction of operator bases of dimension 7 and 8 follows the same manner, for which the SMEFT operator bases at dimension 6 and 7 are needed [87, 88]. For completeness, the axion-dependent renormalisable operators can be found in Eq. (7.21).

$V(a,H)$		aX^2	
$\mathcal{O}_{a^5}$	a^5	$\mathcal{O}_{aB}$	$aB_{\mu\nu}B^{\mu\nu}$
$\mathcal{O}_{a^3H^2}$	$a^3\|H\|^2$	$\mathcal{O}_{a\tilde{B}}$	$aB_{\mu\nu}\widetilde{B}^{\mu\nu}$
$\mathcal{O}_{aH^4}$	$a\|H\|^4$	$\mathcal{O}_{aW}$	$aW^I_{\mu\nu}W^{I,\mu\nu}$
$a\psi^2H + \text{h.c.}$		$\mathcal{O}_{a\tilde{W}}$	$aW^I_{\mu\nu}\widetilde{W}^{I,\mu\nu}$
$\mathcal{O}_{ae}$	$a\bar{L}He$	$\mathcal{O}_{aG}$	$aG^a_{\mu\nu}G^{a,\mu\nu}$
$\mathcal{O}_{au}$	$a\bar{Q}\tilde{H}u$	$\mathcal{O}_{a\tilde{G}}$	$aG^a_{\mu\nu}\widetilde{G}^{a,\mu\nu}$
$\mathcal{O}_{ad}$	$a\bar{Q}Hd$		

Table 7.7: Operators in the aSMEFT at mass dimension 5 with a as a building block.

7.B Operator Basis for the aLEFT up to Mass Dimension 8

7.B.1 With Shift Symmetry

By setting $N_{u,d,\nu,e} \to 1$ and restoring the vanishing terms, the reduced Hilbert series for operator basis up to dimension 8 are given by

$$\begin{aligned}
\mathcal{H}_5^{\text{aLEFT}_{\text{PQ}}} &= 7\partial a\,\psi^2 + 2aX^2\,, \quad \mathcal{H}_6^{\text{aLEFT}_{\text{PQ}}} = 0\,, \quad \mathcal{H}_7^{\text{aLEFT}_{\text{PQ}}} = 8(\partial a)^2\psi^2 + 22\,\partial a\,\psi^2 X\,,\\
\mathcal{H}_8^{\text{aLEFT}_{\text{PQ}}} &= (\partial a)^4 + 7(\partial a)^2\psi^2\mathcal{D} + 6(\partial a)^2X^2 + 32\partial a\,\psi^2X\mathcal{D} + 176\partial a\,\psi^4 + \{6\partial a\,\psi^4\}\,.
\end{aligned} \tag{7.54}$$

The dimension-5 and dimension-7 operator bases are given in Tab. 7.8 and Tab. 7.9 respectively, while the dimension-8 operator basis is presented in Tabs. 7.10, 7.11 and 7.12.

$\partial a\,\psi^2$		$\partial a\,\psi^2$ (cont.)	
$\mathcal{O}^{VL}_{\partial ae}$	$\partial_\mu a\,(\bar{e}_L\gamma^\mu e_L)$	$\mathcal{O}^{VL}_{\partial ad}$	$\partial_\mu a\,(\bar{d}_L\gamma^\mu d_L)$
$\mathcal{O}^{VR}_{\partial ae}$	$\partial_\mu a\,(\bar{e}_R\gamma^\mu e_R)$	$\mathcal{O}^{VR}_{\partial ad}$	$\partial^\mu a\,(\bar{d}_R\gamma^\mu d_R)$
$\mathcal{O}^{VL}_{\partial a\nu}$	$\partial_\mu a\,(\bar{\nu}_L\gamma^\mu \nu_L)$	aX^2	
$\mathcal{O}^{VL}_{\partial au}$	$\partial_\mu a\,(\bar{u}_L\gamma^\mu u_L)$	$\mathcal{O}_{a\tilde{F}}$	$aF_{\mu\nu}\widetilde{F}^{\mu\nu}$
$\mathcal{O}^{VR}_{\partial au}$	$\partial_\mu a\,(\bar{u}_R\gamma^\mu u_R)$	$\mathcal{O}_{a\tilde{G}}$	$aG^a_{\mu\nu}\widetilde{G}^{a,\mu\nu}$

Table 7.8: Operators in the aLEFT at mass dimension 5 with ∂a as a building block. Note that imposing lepton and baryon number conservation, 3 flavour-diagonal entries of the operators coupling the ALP to leptons and quarks, for instance $\mathcal{O}^{VL}_{\partial ae,ii}$, $\mathcal{O}^{VL}_{\partial au,ii}$ and $\mathcal{O}^{VL}_{\partial ad,ii}$, can be removed [176]. Furthermore, we have used that the shift in the operators of class aX^2 can be removed using anomalous chiral transformations on the fermion fields making the operators shift-symmetric without an explicit derivative on the axion field.

$(\partial a)^2\psi^2 + \text{h.c.}$		$\partial a\, X\psi^2$ (cont.)	
$\mathcal{O}^{SR}_{\partial a^2 e}$	$\partial_\mu a\partial^\mu a\,(\bar{e}_L e_R)$	$\mathcal{O}^{VR}_{\partial au\tilde{F}}$	$\partial^\mu a\,(\bar{u}_R\gamma^\nu u_R)\,\widetilde{F}_{\mu\nu}$
$\mathcal{O}^{SR}_{\partial a^2 \nu}$ ($\not{L}$)	$\partial_\mu a\partial^\mu a\,(\bar{\nu}_L \nu^c_L)$	$\mathcal{O}^{VL}_{\partial adF}$	$\partial^\mu a\,(\bar{d}_L\gamma^\nu d_L)\,F_{\mu\nu}$
$\mathcal{O}^{SR}_{\partial a^2 u}$	$\partial_\mu a\partial^\mu a\,(\bar{u}_L u_R)$	$\mathcal{O}^{VR}_{\partial adF}$	$\partial^\mu a\,(\bar{d}_R\gamma^\nu d_R)\,F_{\mu\nu}$
$\mathcal{O}^{SR}_{\partial a^2 d}$	$\partial_\mu a\partial^\mu a\,(\bar{d}_L d_R)$	$\mathcal{O}^{VL}_{\partial ad\tilde{F}}$	$\partial^\mu a\,(\bar{d}_L\gamma^\nu d_L)\,\widetilde{F}_{\mu\nu}$
$\partial a\, X\psi^2$		$\mathcal{O}^{VR}_{\partial ad\tilde{F}}$	$\partial^\mu a\,(\bar{d}_R\gamma^\nu d_R)\,\widetilde{F}_{\mu\nu}$
$\mathcal{O}^{VL}_{\partial aeF}$	$\partial^\mu a\,(\bar{e}_L\gamma^\nu e_L)\,F_{\mu\nu}$	$\mathcal{O}^{VL}_{\partial auG}$	$\partial^\mu a\,(\bar{u}_L\gamma^\nu T^a u_L)\,G^a_{\mu\nu}$
$\mathcal{O}^{VR}_{\partial aeF}$	$\partial^\mu a\,(\bar{e}_R\gamma^\nu e_R)\,F_{\mu\nu}$	$\mathcal{O}^{VR}_{\partial auG}$	$\partial^\mu a\,(\bar{u}_R\gamma^\nu T^a u_R)\,G^a_{\mu\nu}$
$\mathcal{O}^{VL}_{\partial ae\tilde{F}}$	$\partial^\mu a\,(\bar{e}_L\gamma^\nu e_L)\,\widetilde{F}_{\mu\nu}$	$\mathcal{O}^{VL}_{\partial au\tilde{G}}$	$\partial^\mu a\,(\bar{u}_L\gamma^\nu T^a u_L)\,\widetilde{G}^a_{\mu\nu}$
$\mathcal{O}^{VR}_{\partial ae\tilde{F}}$	$\partial^\mu a\,(\bar{e}_R\gamma^\nu e_R)\,\widetilde{F}_{\mu\nu}$	$\mathcal{O}^{VR}_{\partial au\tilde{G}}$	$\partial^\mu a\,(\bar{u}_R\gamma^\nu T^a u_R)\,\widetilde{G}^a_{\mu\nu}$
$\mathcal{O}^{VL}_{\partial a\nu F}$	$\partial^\mu a\,(\bar{\nu}_L\gamma^\nu \nu_L)\,F_{\mu\nu}$	$\mathcal{O}^{VL}_{\partial adG}$	$\partial^\mu a\,(\bar{d}_L\gamma^\nu T^a d_L)\,G^a_{\mu\nu}$
$\mathcal{O}^{VL}_{\partial a\nu\tilde{F}}$	$\partial^\mu a\,(\bar{\nu}_L\gamma^\nu \nu_L)\,\widetilde{F}_{\mu\nu}$	$\mathcal{O}^{VR}_{\partial adG}$	$\partial^\mu a\,(\bar{d}_R\gamma^\nu T^a d_R)\,G^a_{\mu\nu}$
$\mathcal{O}^{VL}_{\partial auF}$	$\partial^\mu a\,(\bar{u}_L\gamma^\nu u_L)\,F_{\mu\nu}$	$\mathcal{O}^{VL}_{\partial ad\tilde{G}}$	$\partial^\mu a\,(\bar{d}_L\gamma^\nu T^a d_L)\,\widetilde{G}^a_{\mu\nu}$
$\mathcal{O}^{VR}_{\partial auF}$	$\partial^\mu a\,(\bar{u}_R\gamma^\nu u_R)\,F_{\mu\nu}$	$\mathcal{O}^{VR}_{\partial ad\tilde{G}}$	$\partial^\mu a\,(\bar{d}_R\gamma^\nu T^a d_R)\,\widetilde{G}^a_{\mu\nu}$
$\mathcal{O}^{VL}_{\partial au\tilde{F}}$	$\partial^\mu a\,(\bar{u}_L\gamma^\nu u_L)\,\widetilde{F}_{\mu\nu}$		

Table 7.9: Operators in the aLEFT at mass dimension 7 with ∂a as a building block. The lepton number violating operator $\mathcal{O}^{LR}_{\partial a^2\nu}$ is marked with ($\not{L}$).

$\partial a\,\psi^4 + \text{h.c.}$		$\partial a\,\psi^4 + \text{h.c.}$ (cont.)	
$\mathcal{O}^{VL,SR}_{\partial aee}$	$\partial_\mu a\,(\bar{e}_L\gamma^\mu e_L)(\bar{e}_L e_R)$	$\mathcal{O}^{VL,TR}_{\partial aeu}$	$\partial_\mu a\,(\bar{e}_L\gamma_\nu e_L)(\bar{u}_L\sigma^{\mu\nu}u_R)$
$\mathcal{O}^{VR,SR}_{\partial aee}$	$\partial_\mu a\,(\bar{e}_R\gamma^\mu e_R)(\bar{e}_L e_R)$	$\mathcal{O}^{VR,SR}_{\partial aeu}$	$\partial_\mu a\,(\bar{e}_R\gamma^\mu e_R)(\bar{u}_L u_R)$
$\mathcal{O}^{VL1,SR}_{\partial auu}$	$\partial_\mu a\,(\bar{u}_L\gamma^\mu u_L)(\bar{u}_L u_R)$	$\mathcal{O}^{VR,TR}_{\partial aeu}$	$\partial_\mu a\,(\bar{e}_R\gamma_\nu e_R)(\bar{u}_L\sigma^{\mu\nu}u_R)$
$\mathcal{O}^{VL8,SR}_{\partial auu}$	$\partial_\mu a\,(\bar{u}_L\gamma^\mu T^a u_L)(\bar{u}_L T^a u_R)$	$\mathcal{O}^{VL,SR}_{\partial aed}$	$\partial_\mu a\,(\bar{e}_L\gamma^\mu e_L)(\bar{d}_L d_R)$
$\mathcal{O}^{VR1,SR}_{\partial auu}$	$\partial_\mu a\,(\bar{u}_R\gamma^\mu u_R)(\bar{u}_L u_R)$	$\mathcal{O}^{VL,TR}_{\partial aed}$	$\partial_\mu a\,(\bar{e}_L\gamma_\nu e_L)(\bar{d}_L\sigma^{\mu\nu}d_R)$
$\mathcal{O}^{VR8,SR}_{\partial auu}$	$\partial_\mu a\,(\bar{u}_R\gamma^\mu T^a u_R)(\bar{u}_L T^a u_R)$	$\mathcal{O}^{VR,SR}_{\partial aed}$	$\partial_\mu a\,(\bar{e}_R\gamma^\mu e_R)(\bar{d}_L d_R)$
$\mathcal{O}^{VL1,SR}_{\partial add}$	$\partial_\mu a\,(\bar{d}_L\gamma^\mu d_L)(\bar{d}_L d_R)$	$\mathcal{O}^{VR,TR}_{\partial aed}$	$\partial_\mu a\,(\bar{e}_R\gamma_\nu e_R)(\bar{d}_L\sigma^{\mu\nu}d_R)$
$\mathcal{O}^{VL8,SR}_{\partial add}$	$\partial_\mu a\,(\bar{d}_L\gamma^\mu T^a d_L)(\bar{d}_L T^a d_R)$	$\mathcal{O}^{VL,SR}_{\partial aue}$	$\partial_\mu a\,(\bar{u}_L\gamma^\mu u_L)(\bar{e}_L e_R)$
$\mathcal{O}^{VR1,SR}_{\partial add}$	$\partial_\mu a\,(\bar{d}_R\gamma^\mu d_R)(\bar{d}_L d_R)$	$\mathcal{O}^{VL,TR}_{\partial aue}$	$\partial_\mu a\,(\bar{u}_L\gamma_\nu u_L)(\bar{e}_L\sigma^{\mu\nu}e_R)$
$\mathcal{O}^{VR8,SR}_{\partial add}$	$\partial_\mu a\,(\bar{d}_R\gamma^\mu T^a d_R)(\bar{d}_L T^a d_R)$	$\mathcal{O}^{VR,SR}_{\partial aue}$	$\partial_\mu a\,(\bar{u}_R\gamma^\mu u_R)(\bar{e}_L e_R)$
$\mathcal{O}^{VL,SR}_{\partial a\nu e}$	$\partial_\mu a\,(\bar{\nu}_L\gamma^\mu \nu_L)(\bar{e}_L e_R)$	$\mathcal{O}^{VR,TR}_{\partial aue}$	$\partial_\mu a\,(\bar{u}_R\gamma_\nu u_R)(\bar{e}_L\sigma^{\mu\nu}e_R)$
$\mathcal{O}^{VL,TR}_{\partial a\nu e}$	$\partial_\mu a\,(\bar{\nu}_L\gamma_\nu \nu_L)(\bar{e}_L\sigma^{\mu\nu}e_R)$	$\mathcal{O}^{VL,SR}_{\partial ade}$	$\partial_\mu a\,(\bar{d}_L\gamma^\mu d_L)(\bar{e}_L e_R)$
$\mathcal{O}^{VL1,SR}_{\partial aud}$	$\partial_\mu a\,(\bar{u}_L\gamma^\mu u_L)(\bar{d}_L d_R)$	$\mathcal{O}^{VL,TR}_{\partial ade}$	$\partial_\mu a\,(\bar{d}_L\gamma_\nu d_L)(\bar{e}_L\sigma^{\mu\nu}e_R)$
$\mathcal{O}^{VL8,SR}_{\partial aud}$	$\partial_\mu a\,(\bar{u}_L\gamma^\mu T^a u_L)(\bar{d}_L T^a d_R)$	$\mathcal{O}^{VR,SR}_{\partial ade}$	$\partial_\mu a\,(\bar{d}_R\gamma^\mu d_R)(\bar{e}_L e_R)$
$\mathcal{O}^{VL1,TR}_{\partial aud}$	$\partial_\mu a\,(\bar{u}_L\gamma_\nu u_L)(\bar{d}_L\sigma^{\mu\nu}d_R)$	$\mathcal{O}^{VR,TR}_{\partial ade}$	$\partial_\mu a\,(\bar{d}_R\gamma_\nu d_R)(\bar{e}_L\sigma^{\mu\nu}e_R)$
$\mathcal{O}^{VL8,TR}_{\partial aud}$	$\partial_\mu a\,(\bar{u}_L\gamma_\nu T^a u_L)(\bar{d}_L\sigma^{\mu\nu}T^a d_R)$	$\mathcal{O}^{VL,SR}_{\partial a\nu u}$	$\partial_\mu a\,(\bar{\nu}_L\gamma^\mu \nu_L)(\bar{u}_L u_R)$
$\mathcal{O}^{VR1,SR}_{\partial aud}$	$\partial_\mu a\,(\bar{u}_R\gamma^\mu u_R)(\bar{d}_L d_R)$	$\mathcal{O}^{VL,TR}_{\partial a\nu u}$	$\partial_\mu a\,(\bar{\nu}_L\gamma_\nu \nu_L)(\bar{u}_L\sigma^{\mu\nu}u_R)$
$\mathcal{O}^{VR8,SR}_{\partial aud}$	$\partial_\mu a\,(\bar{u}_R\gamma^\mu T^a u_R)(\bar{d}_L T^a d_R)$	$\mathcal{O}^{VL,SR}_{\partial a\nu d}$	$\partial_\mu a\,(\bar{\nu}_L\gamma^\mu \nu_L)(\bar{d}_L d_R)$
$\mathcal{O}^{VR1,TR}_{\partial aud}$	$\partial_\mu a\,(\bar{u}_R\gamma_\nu u_R)(\bar{d}_L\sigma^{\mu\nu}d_R)$	$\mathcal{O}^{VL,TR}_{\partial a\nu d}$	$\partial_\mu a\,(\bar{\nu}_L\gamma_\nu \nu_L)(\bar{d}_L\sigma^{\mu\nu}d_R)$
$\mathcal{O}^{VR8,TR}_{\partial aud}$	$\partial_\mu a\,(\bar{u}_R\gamma_\nu T^a u_R)(\bar{d}_L\sigma^{\mu\nu}T^a d_R)$	$\mathcal{O}^{VL,SR}_{\partial adu\nu e}$	$\partial_\mu a\,(\bar{d}_L\gamma^\mu u_L)(\bar{\nu}_L e_R)$
$\mathcal{O}^{VL1,SR}_{\partial adu}$	$\partial_\mu a\,(\bar{d}_L\gamma^\mu d_L)(\bar{u}_L u_R)$	$\mathcal{O}^{VL,SR}_{\partial a\nu ude}$	$\partial_\mu a\,(\bar{\nu}_L\gamma^\mu u_L)(\bar{d}_L e_R)$
$\mathcal{O}^{VL8,SR}_{\partial adu}$	$\partial_\mu a\,(\bar{d}_L\gamma^\mu T^a d_L)(\bar{u}_L T^a u_R)$	$\mathcal{O}^{VR,SR}_{\partial adu\nu e}$	$\partial_\mu a\,(\bar{d}_R\gamma^\mu u_R)(\bar{\nu}_L e_R)$
$\mathcal{O}^{VL1,TR}_{\partial adu}$	$\partial_\mu a\,(\bar{d}_L\gamma_\nu d_L)(\bar{u}_L\sigma^{\mu\nu}u_R)$	$\mathcal{O}^{VR,SR}_{\partial ade\nu u}$	$\partial_\mu a\,(\bar{d}_R\gamma^\mu e_R)(\bar{\nu}_L u_R)$
$\mathcal{O}^{VL8,TR}_{\partial adu}$	$\partial_\mu a\,(\bar{d}_L\gamma_\nu T^a d_L)(\bar{u}_L\sigma^{\mu\nu}T^a u_R)$	$(\partial a)^2 X^2$	
$\mathcal{O}^{VR1,SR}_{\partial adu}$	$\partial_\mu a\,(\bar{d}_R\gamma^\mu d_R)(\bar{u}_L u_R)$	$\mathcal{O}^{(1)}_{\partial a^2 F}$	$\partial_\mu a\partial^\mu a\,F_{\nu\rho}F^{\nu\rho}$
$\mathcal{O}^{VR8,SR}_{\partial adu}$	$\partial_\mu a\,(\bar{d}_R\gamma^\mu T^a d_R)(\bar{u}_L T^a u_R)$	$\mathcal{O}^{(2)}_{\partial a^2 F}$	$\partial_\mu a\partial^\nu a\,F^{\mu\rho}F_{\nu\rho}$
$\mathcal{O}^{VR1,TR}_{\partial adu}$	$\partial_\mu a\,(\bar{d}_R\gamma_\nu d_R)(\bar{u}_L\sigma^{\mu\nu}u_R)$	$\mathcal{O}_{\partial a^2 \tilde{F}}$	$\partial_\mu a\partial^\mu a\,F_{\nu\rho}\widetilde{F}^{\nu\rho}$
$\mathcal{O}^{VR8,TR}_{\partial adu}$	$\partial_\mu a\,(\bar{d}_R\gamma_\nu T^a d_R)(\bar{u}_L\sigma^{\mu\nu}T^a u_R)$	$\mathcal{O}^{(1)}_{\partial a^2 G}$	$\partial_\mu a\partial^\mu a\,G^a_{\nu\rho}G^{a,\nu\rho}$
$\mathcal{O}^{VL,SR}_{\partial aeu}$	$\partial_\mu a\,(\bar{e}_L\gamma^\mu e_L)(\bar{u}_L u_R)$	$\mathcal{O}^{(2)}_{\partial a^2 G}$	$\partial_\mu a\partial^\nu a\,G^{a,\mu\rho}G^a_{\nu\rho}$
$\mathcal{O}^{VL,SR}_{\partial au\nu ed}$	$\partial_\mu a\,(\bar{u}_L\gamma^\mu \nu_L)(\bar{e}_L d_R)$	$\mathcal{O}_{\partial a^2 \tilde{G}}$	$\partial_\mu a\partial^\mu a\,G^a_{\nu\rho}\widetilde{G}^{a,\nu\rho}$
$\mathcal{O}^{VL,SR}_{\partial ae\nu ud}$	$\partial_\mu a\,(\bar{e}_L\gamma^\mu \nu_L)(\bar{u}_L d_R)$	$(\partial a)^4$	
$\mathcal{O}^{VL,SR}_{\partial ade\nu u}$	$\partial_\mu a\,(\bar{d}_L\gamma^\mu e_L)(\bar{\nu}_L u_R)$	$\mathcal{O}_{\partial a^4}$	$\partial_\mu a\partial^\mu a\partial_\nu a\partial^\nu a$
$\mathcal{O}^{VL,SR}_{\partial a\nu edu}$	$\partial_\mu a\,(\bar{\nu}_L\gamma^\mu e_L)(\bar{d}_L u_R)$		

Table 7.10: Operators in the aLEFT at mass dimension 8 with ∂a as a building block.

$(\partial a)^2\psi^2 D$		$\partial a\,\psi^2 XD + \text{h.c. (cont.)}$	
$\mathcal{O}^{VL}_{\partial a^2 eD}$	$\partial_\mu a\partial_\nu a\left(\bar{e}_L\gamma^\mu \overleftrightarrow{D}^\nu e_L\right)$	$\mathcal{O}^{TR}_{\partial aFuD}$	$\partial_\mu a\, F_{\nu\rho}\,(\bar{u}_L\sigma^{\mu\nu}D^\rho u_R)$
$\mathcal{O}^{VR}_{\partial a^2 eD}$	$\partial_\mu a\partial_\nu a\left(\bar{e}_R\gamma^\mu \overleftrightarrow{D}^\nu e_R\right)$	$\mathcal{O}^{SR}_{\partial a\tilde{F}uD}$	$\partial_\mu a\, \widetilde{F}^{\mu\nu}\,(\bar{u}_L D_\nu u_R)$
$\mathcal{O}^{VL}_{\partial a^2 \nu D}$	$\partial_\mu a\partial_\nu a\left(\bar{\nu}_L\gamma^\mu \overleftrightarrow{D}^\nu \nu_L\right)$	$\mathcal{O}^{SR}_{\partial aFdD}$	$\partial_\mu a\, F^{\mu\nu}\left(\bar{d}_L D_\nu d_R\right)$
$\mathcal{O}^{VL}_{\partial a^2 uD}$	$\partial_\mu a\partial_\nu a\left(\bar{u}_L\gamma^\mu \overleftrightarrow{D}^\nu u_L\right)$	$\mathcal{O}^{TR}_{\partial aFdD}$	$\partial_\mu a\, F_{\nu\rho}\left(\bar{d}_L\sigma^{\mu\nu}D^\rho d_R\right)$
$\mathcal{O}^{VR}_{\partial a^2 uD}$	$\partial_\mu a\partial_\nu a\left(\bar{u}_R\gamma^\mu \overleftrightarrow{D}^\nu u_R\right)$	$\mathcal{O}^{SR}_{\partial a\tilde{F}dD}$	$\partial_\mu a\, \widetilde{F}^{\mu\nu}\left(\bar{d}_L D_\nu d_R\right)$
$\mathcal{O}^{VL}_{\partial a^2 dD}$	$\partial_\mu a\partial_\nu a\left(\bar{d}_L\gamma^\mu \overleftrightarrow{D}^\nu d_L\right)$	$\mathcal{O}^{SR}_{\partial aGuD}$	$\partial_\mu a\, G^{a,\mu\nu}\,(\bar{u}_L T^a D_\nu u_R)$
$\mathcal{O}^{VR}_{\partial a^2 dD}$	$\partial_\mu a\partial_\nu a\left(\bar{d}_R\gamma^\mu \overleftrightarrow{D}^\nu d_R\right)$	$\mathcal{O}^{TR}_{\partial aGuD}$	$\partial_\mu a\, G^a_{\nu\rho}\,(\bar{u}_L\sigma^{\mu\nu}T^a D^\rho u_R)$
$\partial a\,\psi^2 XD + \text{h.c.}$		$\mathcal{O}^{SR}_{\partial a\tilde{G}uD}$	$\partial_\mu a\, \widetilde{G}^{a,\mu\nu}\,(\bar{u}_L T^a D_\nu u_R)$
$\mathcal{O}^{SR}_{\partial aFeD}$	$\partial_\mu a\, F^{\mu\nu}\,(\bar{e}_L D_\nu e_R)$	$\mathcal{O}^{SR}_{\partial aGdD}$	$\partial_\mu a\, G^{a,\mu\nu}\left(\bar{d}_L T^a D_\nu d_R\right)$
$\mathcal{O}^{TR}_{\partial aFeD}$	$\partial_\mu a\, F_{\nu\rho}\,(\bar{e}_L\sigma^{\mu\nu}D^\rho e_R)$	$\mathcal{O}^{TR}_{\partial aGdD}$	$\partial_\mu a\, G^a_{\nu\rho}\left(\bar{d}_L\sigma^{\mu\nu}T^a D^\rho d_R\right)$
$\mathcal{O}^{SR}_{\partial a\tilde{F}eD}$	$\partial_\mu a\, \widetilde{F}^{\mu\nu}\,(\bar{e}_L D_\nu e_R)$	$\mathcal{O}^{SR}_{\partial a\tilde{G}dD}$	$\partial_\mu a\, \widetilde{G}^{a,\mu\nu}\left(\bar{d}_L T^a D_\nu d_R\right)$
$\mathcal{O}^{SR}_{\partial aFuD}$	$\partial_\mu a\, F^{\mu\nu}\,(\bar{u}_L D_\nu u_R)$		

Table 7.11: Operators in the aLEFT at mass dimension 8 with ∂a as a building block. [Tab. 7.10 continued.]

$\not{B}$ and $\not{L}$ terms			
$\partial a\, \psi^4 + \text{h.c.}$		$\partial a\, \psi^4 + \text{h.c.}$ (cont.)	
$\mathcal{O}^{VL,SR}_{\partial a e\nu}$	$\partial_\mu a\ (\bar{e}_L \gamma^\mu e_L)\,(\bar{\nu}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a eudu}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{e}^c_R \gamma^\mu u_{L,\alpha})\,(\bar{d}^c_{R,\beta} u_{R,\gamma})$
$\mathcal{O}^{VR,SR}_{\partial a e\nu}$	$\partial_\mu a\ (\bar{e}_R \gamma^\mu e_R)\,(\bar{\nu}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a dueu}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}^c_{R,\alpha} \gamma^\mu u_{L,\beta})\,(\bar{e}^c_R u_{R,\gamma})$
$\mathcal{O}^{VL,SR}_{\partial a u\nu}$	$\partial_\mu a\ (\bar{u}_L \gamma^\mu u_L)\,(\bar{\nu}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a uude}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{u}_{L,\alpha} \gamma^\mu u^c_{R,\beta})\,(\bar{d}_{L,\gamma} e^c_L)$
$\mathcal{O}^{VR,SR}_{\partial a u\nu}$	$\partial_\mu a\ (\bar{u}_R \gamma^\mu u_R)\,(\bar{\nu}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a duue}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}_{L,\alpha} \gamma^\mu u^c_{R,\beta})\,(\bar{u}_{L,\gamma} e^c_L)$
$\mathcal{O}^{VL,SR}_{\partial a d\nu}$	$\partial_\mu a\ (\bar{d}_L \gamma^\mu d_L)\,(\bar{\nu}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a ueud}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{u}_{L,\alpha} \gamma^\mu e^c_R)\,(\bar{u}_{L,\beta} d^c_{L,\gamma})$
$\mathcal{O}^{VR,SR}_{\partial a d\nu}$	$\partial_\mu a\ (\bar{d}_R \gamma^\mu d_R)\,(\bar{\nu}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a udue}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{u}_{L,\alpha} \gamma^\mu d^c_{R,\beta})\,(\bar{u}_{L,\gamma} e^c_L)$
$\mathcal{O}^{VL,SR}_{\partial a ude\nu}$	$\partial_\mu a\ (\bar{u}_L \gamma^\mu d_L)\,(\bar{e}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a \nu ddu}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{\nu}_L \gamma^\mu d^c_{R,\alpha})\,(\bar{d}_{L,\beta} u^c_{L,\gamma})$
$\mathcal{O}^{VL,SR}_{\partial a edu\nu}$	$\partial_\mu a\ (\bar{e}_L \gamma^\mu d_L)\,(\bar{u}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a dd\nu u}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}_{L,\alpha} \gamma^\mu d^c_{R,\beta})\,(\bar{\nu}_L u^c_{L,\gamma})$
$\mathcal{O}^{VL,SR}_{\partial a eu\nu d}$	$\partial_\mu a\ (\bar{e}_L \gamma^\mu u^c_R)\,(\bar{\nu}_L d_R)$	$\mathcal{O}^{VL,SR}_{\partial a d\nu ud}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}_{L,\alpha} \gamma^\mu \nu_L)\,(\bar{u}_{L,\beta} d^c_{L,\gamma})$
$\mathcal{O}^{VL,SR}_{\partial a \nu ued}$	$\partial_\mu a\ (\bar{\nu}_L \gamma^\mu u^c_R)\,(\bar{e}_L d_R)$	$\mathcal{O}^{VR,SR}_{\partial a ud\nu d}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{u}^c_{L,\alpha} \gamma^\mu d_{R,\beta})\,(\bar{\nu}_L d_{R,\gamma})$
$\mathcal{O}^{VL,SR}_{\partial a \nu eud}$	$\partial_\mu a\ (\bar{\nu}_L \gamma^\mu e^c_R)\,(\bar{u}_L d_R)$	$\mathcal{O}^{VL,SR}_{\partial a d\nu du}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}^c_{R,\alpha} \gamma^\mu \nu_L)\,(\bar{d}^c_{R,\beta} u_{R,\gamma})$
$\mathcal{O}^{VL,SR}_{\partial a ue\nu d}$	$\partial_\mu a\ (\bar{u}_L \gamma^\mu e^c_R)\,(\bar{\nu}_L d_R)$	$\mathcal{O}^{VL,SR}_{\partial a dud\nu}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}_{L,\alpha} \gamma^\mu u^c_{R,\beta})\,(\bar{d}_{L,\gamma} \nu^c_L)$
$\mathcal{O}^{VR,SR}_{\partial a \nu edu}$	$\partial_\mu a\,(\bar{\nu}^c_L \gamma^\mu e_R)\,(\bar{d}_L u_R)$	$\mathcal{O}^{VR,SR}_{\partial a dd\nu u}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}^c_{L,\alpha} \gamma^\mu d_{R,\beta})\,(\bar{\nu}_L u_{R,\gamma})$
$\mathcal{O}^{VR,SR}_{\partial a \nu ude}$	$\partial_\mu a\,(\bar{\nu}^c_L \gamma^\mu u_R)\,(\bar{d}_L e_R)$	$\mathcal{O}^{VR,SR}_{\partial a du\nu d}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}^c_{L,\alpha} \gamma^\mu u_{R,\beta})\,(\bar{\nu}_L d_{R,\gamma})$
$\mathcal{O}^{VL,SR}_{\partial a \nu}$ $(\star)$	$\partial_\mu a\ (\bar{\nu}_L \gamma^\mu \nu_L)\,(\bar{\nu}_L \nu^c_L)$	$\mathcal{O}^{VL,SR}_{\partial a dedd}$ $(\star)$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}^c_{R,\alpha} \gamma^\mu e_L)\,(\bar{d}_{L,\beta} d^c_{L,\gamma})$
$\mathcal{O}^{VR,SR}_{\partial a dded}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}^c_{L,\alpha} \gamma^\mu d_{R,\beta})\,(\bar{e}_L d_{R,\gamma})$	$\mathcal{O}^{VR,SR}_{\partial a eddd}$ $(\star)$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{e}_R \gamma^\mu d_{R,\alpha})\,(\bar{d}^c_{R,\beta} d_{R,\gamma})$
$\mathcal{O}^{VL,SR}_{\partial a ddde}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}_{L,\alpha} \gamma^\mu d^c_{R,\beta})\,(\bar{d}_{L,\gamma} e_R)$	$\partial a\, \psi^2 X D + \text{h.c.}$	
$\mathcal{O}^{VR,SR}_{\partial a euud}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{e}^c_L \gamma^\mu u_{R,\alpha})\,(\bar{u}^c_{R,\beta} d_{R,\gamma})$	$\mathcal{O}^{SR}_{\partial a F\nu D}$	$\partial_\mu a\, F^{\mu\nu}\,(\bar{\nu}_L \sigma_{\nu\rho} \partial^\rho \nu^c_L)$
$\mathcal{O}^{VR,SR}_{\partial a duue}$	$\partial_\mu a\, \epsilon^{\alpha\beta\gamma}\,(\bar{d}^c_{L,\alpha} \gamma^\mu u_{R,\beta})\,(\bar{u}^c_{R,\gamma} e_R)$		

Table 7.12: B- and L-breaking operators in the aLEFT at mass dimension 8 with ∂a as a building block. Note that the operators marked with $(\star)$ do not appear when the number of fermion flavours is set to 1. Some errors in the original table published in Ref. [2] have been corrected here thanks to Ref. [330]. [Tab. 7.11 continued].

7.B.2 Without Shift Symmetry

For aLEFT without a shift symmetry, once again, we can use the PQ-breaking isolation condition Eq. (7.34) to construct the operator basis

$$\mathcal{L}_n^{\text{aLEFT}_{\not{\text{PQ}}}} = a\,\mathcal{L}_{n-1}^{\text{aLEFT}_{\not{\text{PQ}}}} + a\,\mathcal{L}_{n-1}^{\text{LEFT}} + \mathcal{L}_n^{\text{aLEFT}_{\text{PQ}}} \tag{7.55}$$

for $n > 5$. As a starting point, we show the operator basis at dimension 5 in Tab. 7.13. The higher-dimensional operator bases can be easily constructed with the LEFT operator bases [291, 318] and the shift-symmetric operator bases. For completeness, the axion-dependent renormalisable operators are shown in Eq. (7.35).

$V(a,H)$		$a^2\psi^2 + \text{h.c.}$	
$\mathcal{O}_{a^5}$	a^5	$\mathcal{O}_{a^2e}^{SR}$	$a^2\bar{e}_L e_R$
aX^2		$\mathcal{O}_{a^2\nu}^{SR}$ ($\not{L}$)	$a^2\bar{\nu}_L\nu_L^c$
$\mathcal{O}_{aF}$	$aF_{\mu\nu}F^{\mu\nu}$	$\mathcal{O}_{a^2u}^{SR}$	$a^2\bar{u}_L u_R$
$\mathcal{O}_{a\tilde{F}}$	$aF_{\mu\nu}\widetilde{F}^{\mu\nu}$	$\mathcal{O}_{a^2d}^{SR}$	$a^2\bar{d}_L d_R$
$\mathcal{O}_{aG}$	$aG^a_{\mu\nu}G^{a,\mu\nu}$		
$\mathcal{O}_{a\tilde{G}}$	$aG^a_{\mu\nu}\widetilde{G}^{a,\mu\nu}$		

Table 7.13: Operators in the aLEFT at mass dimension 5 with a as a building block. It is worth noting that the dimension-5 ALP Yukawa couplings in the aSMEFT in Tab. 7.7 become dimension-4 ALP-dependent mass terms in the aLEFT. The lepton number violating operator $\mathcal{O}_{a^2\nu}$ is marked with ($\not{L}$).

7.C Details on the Basis Change from the Derivative to the Yukawa Basis

Previous discussions of the shift symmetry in the presence of the EOM redundancy at dimension 5 focused on the effect on the leading order interactions and did not take the effect of the field redefinition on higher order operators into consideration. Furthermore, the effect on ALP-independent effective operators built from SM fields are also ignored. In this section, we will study the effect of the field redefinition on those operators.

7.C.1 ALP-Dependent Operators

We will first ignore the SMEFT operators and start with the full derivatively coupled Lagrangian up to dimension-7, i.e., all operators in Tabs. 7.3-7.5. To keep the discussion concise, we only show the calculations for one higher order operator, while the calculations for the other operators follow in a straightforward way. Furthermore, we ignore the bosonic operators here, as they are irrelevant to the discussion[15]. The first derivatively coupled fermionic oper-

[15] Apart from the anomalous dimension 5 operators including gauge fields. Those have been treated previously in the literature.

ators beyond the leading order appears at dimension-7. Eventually, we consider the following Lagrangian

$$\begin{aligned}\mathcal{L} = \sum_{\psi\in\text{SM}} \bar\psi i\not{D}\psi - \left(\bar{Q}Y_u\tilde{H}u + \bar{Q}Y_d H d + \bar{L}Y_e H e + \text{h.c.}\right) + \frac{\partial_\mu a}{f}\sum_{\psi\in\text{SM}}\bar\psi\gamma^\mu C_\psi\psi \\ + \frac{\partial^\mu a}{f^3}\left(\bar{L}\gamma^\nu C_{\partial aLB}L\right)B_{\mu\nu} + \dots\end{aligned} \tag{7.56}$$

where the dots collect all the other terms in the derivatively coupled EFT that follow the same discussion. Redefining the fermion fields by $\psi \to \exp\left(iC_\psi \frac{a}{f}\right)\psi$, trades the derivatively coupled operators at dimension-5 for the ALP-Yukawa couplings but also generates more operators at higher dimensions. We find

$$\begin{aligned}\mathcal{L} \to \sum_{\psi\in\text{SM}} \bar\psi i\not{D}\psi - \cancel{\frac{\partial_\mu a}{f}\sum_{\psi\in\text{SM}}\bar\psi\gamma^\mu C_\psi\psi} - \left(\bar{Q}e^{-iC_Q\frac{a}{f}}Y_u e^{iC_u\frac{a}{f}}\tilde{H}u + \bar{Q}e^{-iC_Q\frac{a}{f}}Y_d e^{iC_d\frac{a}{f}}Hd\right. \\ \left. + \bar{L}e^{-iC_L\frac{a}{f}}Y_e e^{iC_e\frac{a}{f}}He + \text{h.c.}\right) + \cancel{\frac{\partial_\mu a}{f}\sum_{\psi\in\text{SM}}\bar\psi\gamma^\mu C_\psi\psi} + \frac{\partial^\mu a}{f^3}\left(\bar{L}e^{-iC_L\frac{a}{f}}\gamma^\nu C_{\partial aLB}e^{iC_L\frac{a}{f}}L\right)B_{\mu\nu} + \dots\end{aligned} \tag{7.57}$$

Expanding these exponentials in the SM Yukawa couplings to leading order yields the usual relations at dimension-5. Here, we will also study how they alter the dimension-7 operators and the rest of the tower of interactions that is generated by expanding the exponential of the ALP appearing after the field redefinition is performed.

Focusing only on the leptonic terms, we have after expanding the exponentials

$$\begin{aligned}\mathcal{L} \to \sum_{\psi\in\text{SM}} \bar\psi i\not{D}\psi - \bar{L}\left[Y_e + \frac{a}{f}i\left(Y_eC_e - C_LY_e\right) + \frac{a^2}{f^2}\left(C_LY_eC_e - \frac{1}{2}\left(C_L^2Y_e + Y_eC_e^2\right)\right) + \dots\right]He \\ + \frac{\partial^\mu a}{f^3}\left(\bar{L}\gamma^\nu\left[C_{\partial aLB} + \frac{a}{f}i\left(C_{\partial aLB}C_L - C_LC_{\partial aLB}\right) + \frac{a^2}{f^2}\left(C_LC_{\partial aLB}C_L\right.\right.\right. \\ \left.\left.\left. - \frac{1}{2}\left(C_L^2C_{\partial aLB} + C_{\partial aLB}C_L^2\right)\right) + \dots\right]L\right)B_{\mu\nu} + \dots .\end{aligned} \tag{7.58}$$

Notice that expanding the exponential introduces more shift-breaking interactions beyond what is usually shown in the literature. As for the dimension-5 Yukawa couplings, the Wilson coefficients of those shift-breaking operators have to fulfil relations dictated by the exponentiated form of the ALP interactions. We find for the operators shown in the Lagrangian

$$\begin{aligned}C_{ae} &= i\left(C_LY_e - Y_eC_e\right), \\ C_{a^2e} &= \left(\frac{1}{2}\left(C_L^2Y_e + Y_eC_e^2\right) - C_LY_eC_e\right), \\ C_{a\partial aLB} &= i\left(C_{\partial aLB}C_L - C_LC_{\partial aLB}\right), \\ C_{a^2\partial aLB} &= \left(C_LC_{\partial aLB}C_L - \frac{1}{2}\left(C_L^2C_{\partial aLB} + C_{\partial aLB}C_L^2\right)\right),\end{aligned} \tag{7.59}$$

where we have used the notation introduced in App. 7.A.2 for the shift-breaking operators.

Note that the parameter counting in the EFT before and after the field redefinition is still consistent after including the higher order operators as well. At dimension 5, the relations remove the finite difference between the couplings captured in the shift-symmetric and non-shift-symmetric EFTs. At higher mass dimension, the relations fully saturate the freedom in the Wilson coefficients of the shift-breaking operators and no new parameters are added, as expected. This happens due to the exponential generating a tower of interactions proportional to the same Wilson coefficient of the shift-symmetric operator that is affected by the chiral rotation.

In order to obtain a shift-symmetric ALP EFT in the Yukawa basis beyond dimension 5, the additional interactions with fully constrained Wilson coefficients have to be included. Otherwise one will run into shift-breaking results while doing computations. Only when all the additional diagrams from the operators generated by the field redefinitions are considered, one will recover a shift-symmetric result.

7.C.2 SMEFT Operators

The ALP-dependent chiral transformation also affects SMEFT operators, which were previously completely ALP-independent. We will give some examples here, working with the following Lagrangian[16]

$$
\begin{aligned}
\mathcal{L}_{\rm SMEFT} &= \frac{1}{f^2}|H|^2\bar{L}C_{eH}He + \frac{1}{f^2}C^{(1)}_{lequ,ijkl}\left(\bar{L}_i e_j\right)\epsilon\left(\bar{Q}_k u_l\right)\\
&\longrightarrow \frac{|H|^2}{f^2}\bar{L}\left[C_{eH} + \frac{a}{f}i\left(C_{eH}C_e - C_L C_{eH}\right) + \frac{a^2}{f^2}\left(C_L C_{eH} C_e - \frac{1}{2}\left(C_L^2 C_{eH} + C_{eH}C_e^2\right)\right)\right]He\\
&+ \frac{1}{f^2}\left[C^{(1)}_{lequ,ijkl} + \frac{a}{f}i\left(C^{(1)}_{lequ,ij'kl}C_{e,j'j} + C^{(1)}_{lequ,ijkl'}C_{u,l'l} - C^{(1)}_{lequ,i'jkl}C_{L,ii'} - C^{(1)}_{lequ,ijk'l}C_{Q,kk'}\right)\right.\\
&+\frac{a^2}{f^2}\left(C^{(1)}_{lequ,i'j'kl}C_{L,ii'}C_{e,j'j} - C^{(1)}_{lequ,i'jk'l}C_{L,ii'}C_{Q,kk'} + C^{(1)}_{lequ,i'jkl'}C_{L,ii'}C_{u,l'l}\right.\\
&+C^{(1)}_{lequ,ij'k'l}C_{e,j'j}C_{Q,kk'} - C^{(1)}_{lequ,ij'kl'}C_{e,j'j}C_{u,l'l} + C^{(1)}_{lequ,ijk'l'}C_{Q,kk'}C_{u,l'l}\\
&\left.\left.-\frac{1}{2}\left(C^{(1)}_{lequ,i'jkl}(C_L^2)_{ii'} + C^{(1)}_{lequ,ij'kl}(C_e^2)_{j'j} + C^{(1)}_{lequ,ijk'l}(C_Q^2)_{kk'} + C^{(1)}_{lequ,ijkl'}(C_u^2)_{l'l}\right)\right)\right]\times\\
&\times\left(\bar{L}_i e_j\right)\epsilon\left(\bar{Q}_k u_l\right)\,.
\end{aligned}
$$

Comparing to the generic shift-breaking Lagrangian, similar relations are found as before. They become more and more complicated as more fermions appear in the operators. One can simply read off the relations from the Lagrangian and we will not give them explicitly again.

In order to derive these relations one can also start in the aSMEFT$_{\not{PQ}}$, where the shift symmetry is not imposed explicitly, by demanding that a shift of the ALP $a \to a + c$ can be removed by a field redefinitions, while staying in the same operator basis. We have checked explicitly with our operator basis up to dimension-8 that one obtains the same relations this way.

[16]For simplicity we have taken the operators with and without an ALP to be suppressed by the same UV scale f. Depending on the structure of the UV theory and the details of PQ-breaking the operators can also come with a suppression of different scales corresponding to different UV sectors.

To this end, a field redefinition should be used that allows to remove the shift c in the Lagrangian while keeping the kinetic terms of the fermions invariant and at the same time not generating new operators outside of the operator basis we start with. The only such transformation is given by redefining the fermion fields with powers of the shift $\frac{c}{f}$ as $\psi \to \psi + i \sum_{k=1}^{\infty} c_\psi^{(k)} \left(\frac{c}{f}\right)^k \psi$, where the $c_\psi^{(k)}$ are generic hermitian matrices. We keep the terms in this expansion up to the order that is relevant for the EFT expansion in each step of the discussion. Getting consistent relations for all terms that are proportional to the shift for operators with more than one power of an ALP requires the following choice for the coefficients in the field redefinition $c_\psi^{(n)} = i^{n-1} C_\psi/(n!)$, i.e. $\psi \to \exp\left(i C_\psi \frac{c}{f}\right)\psi$. This is reminiscent of the chiral transformation used to change from the derivative to the Yukawa basis.

7.C.3 List of Additional Relations in Yukawa Basis

In this appendix we list all the constrained Wilson coefficients of operators that have to be added in the Yukawa basis up to dimension 8. Due to the length of the relations obtained by performing ALP-dependent chiral rotations on the fermions in SMEFT operators, we restrict ourselves to the operators which are already ALP-dependent before the field redefinition here.

At dimension 5, we find the well-known relations

$$C_{ae} = i\left(C_L Y_e - Y_e C_e\right), \quad C_{au} = i\left(C_Q Y_u - Y_u C_u\right), \quad C_{ad} = i\left(C_Q Y_d - Y_d C_d\right). \tag{7.60}$$

Since at dimension-6 the only existing operator is bosonic, the only relations at this mass-dimension come again from the ALP-Yukawa operators. They read

$$\begin{gathered} C_{a^2e} = \left(\frac{1}{2}\left(C_L^2 Y_e + Y_e C_e^2\right) - C_L Y_e C_e\right), \quad C_{a^2u} = \left(\frac{1}{2}\left(C_Q^2 Y_u + Y_u C_u^2\right) - C_Q Y_u C_u\right), \\ C_{a^2d} = \left(\frac{1}{2}\left(C_Q^2 Y_d + Y_d C_d^2\right) - C_Q Y_d C_d\right). \end{gathered} \tag{7.61}$$

The same is true at dimension-7

$$\begin{aligned} C_{a^3e} &= \frac{i}{6}\left(Y_e C_e^3 - C_L^3 Y_e\right) + \frac{i}{2}\left(C_L^2 Y_e C_e - C_L Y_e C_e^2\right), \\ C_{a^3u} &= \frac{i}{6}\left(Y_u C_u^3 - C_Q^3 Y_u\right) + \frac{i}{2}\left(C_Q^2 Y_u C_u - C_Q Y_u C_u^2\right), \\ C_{a^3d} &= \frac{i}{6}\left(Y_d C_d^3 - C_Q^3 Y_d\right) + \frac{i}{2}\left(C_Q^2 Y_d C_d - C_Q Y_d C_d^2\right). \end{aligned} \tag{7.62}$$

Only at dimension-8 there exist relations introduced by new fermionic operators at dimension-7 reading as follows

$$\begin{aligned} C_{a^4e} &= \frac{1}{6}\left(C_L^3 Y_e C_e + C_L Y_e C_e^3\right) - \frac{1}{4} C_L^2 Y_e C_e^2 - \frac{1}{24}\left(C_L^4 Y_e + Y_e C_e^4\right), \\ C_{a^4u} &= \frac{1}{6}\left(C_Q^3 Y_u C_u + C_Q Y_u C_u^3\right) - \frac{1}{4} C_Q^2 Y_u C_u^2 - \frac{1}{24}\left(C_Q^4 Y_u + Y_u C_u^4\right), \\ C_{a^4d} &= \frac{1}{6}\left(C_Q^3 Y_d C_d + C_Q Y_d C_d^3\right) - \frac{1}{4} C_Q^2 Y_d C_d^2 - \frac{1}{24}\left(C_Q^4 Y_d + Y_d C_d^4\right), \end{aligned}$$

$$
\begin{aligned}
C^{(1,2)}_{a\partial aeHD} &= i\left(C^{(1,2)}_{\partial aeHD}C_e - C_L C^{(1,2)}_{\partial aeHD}\right) , \\
C^{(1,2)}_{a\partial auHD} &= i\left(C^{(1,2)}_{\partial auHD}C_u - C_Q C^{(1,2)}_{\partial auHD}\right) , \\
C^{(1,2)}_{a\partial adHD} &= i\left(C^{(1,2)}_{\partial adHD}C_d - C_L C^{(1,2)}_{\partial adHD}\right) , \\
C_{a\partial a\psi H^2} &= i\left(C_{\partial a\psi H^2}C_\psi - C_\psi C_{\partial a\psi H^2}\right) , \\
C_{a\partial a\psi V} &= i\left(C_{\partial a\psi V}C_\psi - C_\psi C_{\partial a\psi V}\right) .
\end{aligned}
\tag{7.63}
$$

For the last relation, the same relation holds true for the operators with the dual field strength. Furthermore, some shift-symmetric operator at dimension-8 get shifted as follows

$$
\begin{aligned}
C_{\partial a^2 eH} &\to C_{\partial a^2 eH} + i\left(C^{(2)}_{\partial aeHD}C_e - C_L C^{(1)}_{\partial aeHD}\right), \\
C_{\partial a^2 uH} &\to C_{\partial a^2 uH} + i\left(C^{(2)}_{\partial auHD}C_u - C_Q C^{(1)}_{\partial auHD}\right), \\
C_{\partial a^2 dH} &\to C_{\partial a^2 dH} + i\left(C^{(2)}_{\partial adHD}C_d - C_Q C^{(1)}_{\partial adHD}\right),
\end{aligned}
\tag{7.64}
$$

due to the derivative acting on the fermions in the operator corresponding to the last relation in the previous equation.

8

Small Instanton-Induced Flavour Invariants and the Axion Potential

8.1 Introduction

We have introduced the axion solution to the strong CP problem in Sec. 2.4.1. There, we saw that one of the main ingredients of the axion solution to the strong CP problem is the mixed anomaly of the PQ symmetry with QCD. This allows the axion to receive a potential only from non-perturbative QCD effects ensuring that it has a minimum that exactly cancels $\bar{\theta}$. For this to work, one has to implicitly assume that the non-perturbative QCD effects are the dominant source of explicit PQ breaking. Generically, shift symmetry-violating terms (which may be CP-violating) arising from interactions of the axion with gravity spoil the axion solution by misaligning the minimum of the axion potential. These contributions must therefore be sufficiently suppressed, leading to the so-called axion quality problem. However, even under the assumption that the irreducible shift-violating operators in the axion EFT generated by quantum gravity are sufficiently suppressed, another aspect of the axion quality problem concerns non-gravitational effects that can generate a misaligned potential for the axion.

One might ask if the perturbative source of CP violation in the SM already poses a problem to the axion solution by introducing radiative corrections to $\bar{\theta}$, thus misaligning the axion potential. However, it turns out that the corrections induced by the CKM phase, first appear at seven loops [331, 332] through RG running, while finite contributions appear at four loops although still highly suppressed [333]. The high suppression in the SM is due to the flavourful nature of CP violation in the SM, which requires the Lagrangian parameters responsible for CP violation to appear in a specific way, which is invariant under the change of a flavour basis as discussed earlier in this thesis. The problem can be exacerbated considering BSM physics, which can be parameterised in higher-dimensional terms of the SM fields, potentially causing order-one shifts in $\bar{\theta}$ thereby potentially invalidating solutions to the strong CP problem [334]. This has been studied in the context of the SMEFT, where higher-dimensional CP-violating terms induced at a scale $\Lambda_{\not{CP}}$ can shift $\bar{\theta}$ and misalign the axion potential [335–337].

The new sources of CP violation are highly dependent on the specific UV completion.

If the main source of PQ breaking is still due to low-energy QCD effects and only the new source of CP violation arises at a high scale, then the effects on the axion potential and the neutron EDM generically depend on $\frac{\Lambda_{\rm QCD}}{\Lambda_{\not{CP}}}$ and decouple as $\Lambda_{\not{CP}} \to \infty$. Alternatively, there has been renewed interest in the old idea to modify QCD at a UV scale, such that instanton effects breaking the PQ symmetry become relevant at high scales. These small instanton effects, present at a scale $\Lambda_{\rm SI}$ can increase the axion mass while still solving the strong CP problem [239, 240, 335, 338–345]. If in addition to this modification of QCD in the UV there also exist new CP-violating sources, they can also be enhanced by the UV instantons, whose effects are no longer suppressed due to the assumed larger QCD coupling at the scale $\Lambda_{\rm SI}$. These contributions misalign the minimum of the axion potential, where the leading contributions to $\bar{\theta}$ then scale as $\Lambda_{\rm SI}^2/\Lambda_{\not{CP}}^2$ [337] which do not necessarily decouple (i.e. when $\Lambda_{\rm SI}, \Lambda_{\not{CP}} \to \infty$ with a finite ratio $\Lambda_{\rm SI}/\Lambda_{\not{CP}}$) and give rise to important constraints on CP-violating couplings in certain UV scenarios. For a sufficiently small (although large) QCD gauge coupling these effects can be computed by performing a 1-instanton calculation which provides the dominant contribution to the action. However, when the QCD gauge coupling becomes non-perturbative, the dilute instanton gas approximation breaks down and non-perturbative methods must be used.[1]

The effects of CP violation arising from higher-dimensional operators in an instanton background, including a 4-quark SMEFT operator were computed in Refs. [337, 352, 353] and estimated using an instanton naive dimensional analysis (NDA) in Ref. [242]. However, different CP-violating UV scenarios can give rise to many other operators [80, 81] and therefore previous estimates of the contributions to $\bar{\theta}$ should be generalised for the complete list of SMEFT operators.

As discussed throughout this thesis, observable quantities – like contributions to $\bar{\theta}$ – must be independent of the flavour basis, and hence can be written in terms of flavour-invariant quantities constructed from the Wilson coefficients and other renormalisable flavourful couplings. As we will see below, the CP-odd flavour invariants of the SMEFT will allow for an estimation of the physical consequences of the Wilson coefficients – especially when used together with other NDA techniques [242] – prior to any explicit computation. These advantages have been previously been used for physical estimates [257, 331, 332, 354–356].

Besides providing an order parameter to estimate CP-violating physical effects, the CP-odd invariants enable the systematisation of the complicated instanton computations by predicting the form of the contribution of a given Wilson coefficients, such as the number of Yukawa coupling insertions or loop factor suppressions. For example, we will show that semi-leptonic operators generate a $\overline{\theta}$ but are suppressed by one extra loop-order and an extra lepton Yukawa factor compared with 4-quark operators. Furthermore, knowing the number of up, down and lepton Yukawa couplings needed to construct the invariants, we will be able to classify the leading contributions for arbitrary Wilson coefficients. Another advantage of the invariants is the simple application of different flavour scenarios in the given UV completions. Lastly, most computations in the literature have focused on the limit of completely diagonal Yukawa matrices but, which is generalised in a straightforward way to the case of generic Yukawa

[1] All topological configurations contribute equally in the non-perturbative regime. Thus, multi-instanton solutions and the interactions between among the instantons need to be taken into consideration [346–351].

couplings by the use of flavour invariants.

Due to the CP nature of $\bar{\theta}$, the induced $\bar{\theta}$ in the presence of different SMEFT operators can be captured via the CP-violating invariants introduced in Sec. 2.2.3 based on Refs. [103, 104], where a basis of CP-odd flavour invariants was put forward to describe the leading order sources of CP violation in the SMEFT. The invariants introduced there all came in the form of the imaginary part of a trace of flavourful matrices. We will show in this chapter that the invariants appearing in the instanton computations all have determinant-like structures instead of the traces. We will construct a new basis for these determinant-like invariants and show that they can be expressed as complicated combination of CP-even and -odd trace invariants. We will show explicitly that these determinant-like structures naturally arise in a Grassmann integration that appears in the instanton computations.

While the flavour invariants introduced here allow to make estimates for $\bar{\theta}$ induced by CP-violating operators in the SMEFT, we will also perform the detailed computation of $\bar{\theta}$ in the presence of small instantons, showing explicitly how these invariants appear in the computations. In particular, we generalise previous results on the insertion of the CP-violating 4-quark operator $\mathcal{O}^{(1)}_{\rm quqd}$ and calculate the effects of the semi-leptonic, $\mathcal{O}^{(1)}_{\rm lequ}$ and gluon chromo-dipole, $\mathcal{O}_{\rm dG}$ operators. Subsequently, we use the stringent upper bound on $\bar{\theta}$ to set bounds on the Wilson coefficients of the operators in different flavour scenarios improving previous bounds, where the contributions from off-diagonal SM Yukawa couplings were neglected. For the leading order operators, such as the 4-quark and gluon dipole operators, we find that $\Lambda_{\not{CP}} \gtrsim 10^6\,\Lambda_{\rm SI}$, assuming a minimally flavour violating (MFV) scenario for the SMEFT couplings. Under these same flavour assumptions, the loop-suppressed contributions, arising from $\mathcal{O}^{(1)}_{\rm lequ}$, lead to the weaker constraint $\Lambda_{\not{CP}} \gtrsim 10^4\,\Lambda_{\rm SI}$. The bounds become more stringent if there is no flavour structure in the Wilson coefficients, such as the anarchic flavour scenario. In this case, assuming all the Wilson coefficients are of order one, we obtain $\Lambda_{\not{CP}} \gtrsim 10^{11}\,\Lambda_{\rm SI}$ for the 4-quark operator $\mathcal{O}^{(1)}_{\rm quqd}$, $\Lambda_{\not{CP}} \gtrsim 10^8\,\Lambda_{\rm SI}$ for the gluon dipole operator $\mathcal{O}_{\rm dG}$ and $\Lambda_{\not{CP}} \gtrsim 10^7\,\Lambda_{\rm SI}$ for the semi-leptonic operator $\mathcal{O}^{(1)}_{\rm lequ}$.

8.2 Flavour Invariants Featuring $\theta_{\rm QCD}$

The single source of perturbative CP violation in the SM arises as an intricate collective effect that can only be properly described by a combination of Lagrangian parameters. It can be most effectively described by the Jarlskog invariant $J_4 = {\rm Im}\left({\rm Tr}\,[X_{\rm u}, X_{\rm d}]^3\right)$, discussed throughout this thesis, where $X_{\rm u,d} \equiv Y_{\rm u,d} Y^\dagger_{\rm u,d}$. The Jarlskog invariant is the order parameter of perturbative CP violation in the SM as it captures the single physical phase in the renormalisable SM Lagrangian in a flavour basis-invariant way (c.f. Tab. 8.1). Here, we have used the fact that $U(3)^5 \equiv U(3)_{\rm Q} \times U(3)_{\rm u} \times U(3)_{\rm d} \times U(3)_{\rm L} \times U(3)_{\rm e}$ is the largest possible flavour group allowed by the SM fermion kinetic terms and is only broken by the SM Yukawa couplings and global anomalies. The Lagrangian can be formally made invariant under this symmetry by promoting the Yukawa couplings to spurions transforming under $U(3)^5$ as given in the Tab. 8.1.

This discussion can be extended to the non-perturbative source of CP violation in the SM, the QCD θ-angle, which also transforms under the Abelian part of the $U(3)^5$ flavour group

	$U(3)_{\rm Q}$	$U(3)_{\rm u}$	$U(3)_{\rm d}$	$U(3)_{\rm L}$	$U(3)_{\rm e}$
$e^{i\theta_{\rm QCD}}$	$\mathbf{1}_{+6}$	$\mathbf{1}_{-3}$	$\mathbf{1}_{-3}$	$\mathbf{1}_{0}$	$\mathbf{1}_{0}$
$Y_{\rm u}$	$\mathbf{3}_{+1}$	$\bar{\mathbf{3}}_{-1}$	$\mathbf{1}_{0}$	$\mathbf{1}_{0}$	$\mathbf{1}_{0}$
$Y_{\rm d}$	$\mathbf{3}_{+1}$	$\mathbf{1}_{0}$	$\bar{\mathbf{3}}_{-1}$	$\mathbf{1}_{0}$	$\mathbf{1}_{0}$
$Y_{\rm e}$	$\mathbf{1}_{0}$	$\mathbf{1}_{0}$	$\mathbf{1}_{0}$	$\mathbf{3}_{+1}$	$\bar{\mathbf{3}}_{-1}$

Table 8.1: Behaviour of $\theta_{\rm QCD}$ and the Yukawa coupling matrices $Y_{\rm u,d,e}$ under flavour transformation of the SM fermion fields. The subscripts of the $SU(3)$ representations denote the charge under the $U(1)$ part of the flavour symmetry.

(see Tab. 8.1). Given this transformation, the flavour invariant

$$J_\theta = {\rm Im}[e^{-i\theta_{\rm QCD}}\det(Y_{\rm u}Y_{\rm d})]\,, \tag{8.1}$$

captures the *non*-perturbative source of CP violation in the SM Lagrangian,[2] specifically $\bar\theta = \theta_{\rm QCD} + \arg\det[Y_{\rm u}Y_{\rm d}]$. The contribution of the SM Lagrangian in the presence of an instanton background has the following dependence [143, 239]

$$V\left(\theta_{\rm QCD}, Y_{\rm u}, Y_{\rm d}\right) \propto e^{-i\theta_{\rm QCD}}\prod_{i=1}^{3}\hat y_{{\rm u},i}\,\hat y_{{\rm d},i}\,, \tag{8.2}$$

where $\hat y_{{\rm u},i}$, $\hat y_{{\rm d},i}$ are the Yukawa matrix eigenvalues and i labels the quark flavours. Later, the eigenvalues will sometimes be referred to by their particle name, i.e. for instance $\hat y_{{\rm u},3} = y_{\rm t}$. This is reminiscent of the invariant just defined and the flavour dependence of the result can be reproduced from J_θ or $K_\theta = {\rm Re}[e^{-i\theta_{\rm QCD}}\det(Y_{\rm u}Y_{\rm d})]$ (depending on the CP parity of the contribution to V) by expanding the invariants in the limit of diagonal SM Yukawa matrices. This suggests that the flavour invariants can appear directly in instanton calculations provided general flavourful couplings are used in the computation.

In this chapter, we want to consider the contribution of new sources of CP violation in the UV, parameterised by SMEFT operators, to the vacuum energy in the presence of (small) instantons. Therefore, we expect some modified form of the CP-odd SMEFT invariants introduced in Sec. 2.2.3 to show up in the instanton computations. The effect of the 4-fermion operator $\mathcal{O}^{(1)}_{\rm ququd} = \bar Q u \bar Q d$ in the Lagrangian, $\mathcal{L} \supset C^{(1)}_{\rm ququd}\mathcal{O}^{(1)}_{\rm ququd}/\Lambda^2_{\not{CP}}$ on the correlator, $\chi_{\rm ququd}$, in an instanton background, was calculated in Ref. [337] (see Fig. 8.1a). In the limit of diagonal

[2]For instance, the correction to the axion mass in the SM is proportional to $K_\theta = {\rm Re}[e^{-i\theta_{\rm QCD}}\det(Y_{\rm u}Y_{\rm d})] \propto \cos\bar\theta$, leading to the well-known cosine potential [144, 150], whereas the linear term of the axion potential generated via non-perturbative QCD effects in the SM is proportional to $J_\theta \propto \sin\bar\theta$.

SM Yukawa couplings,[3] the contribution has the following form [337]

$$V\left(\theta_{\rm QCD}, Y_{\rm u}, Y_{\rm d}, C^{(1)}_{\rm quqd}\right) \propto e^{-i\theta_{\rm QCD}} \frac{c_{ij}}{\hat{y}_{{\rm u},i}\hat{y}_{{\rm d},j}} \prod_{k=1}^{3} \hat{y}_{{\rm u},k}\hat{y}_{{\rm d},k}\,, \tag{8.3}$$

where c_{ij} labels the two possible flavour structures $c_{ij} = C^{(1)}_{{\rm quqd},iijj}$ or $c_{ij} = C^{(1)}_{{\rm quqd},ijji}$, that can appear in the computations, and k labels the six entries of the diagonal Yukawa matrices. The proportionality factor in Eq. (8.3) depends on the details of the instanton calculation, which we will perform in detail in Sec. 8.3.

From the expression in Eq. (8.3) it is not apparent that the result can be expressed in terms of the previously considered CP-odd trace invariants of the SMEFT. As mentioned in the introduction, determinant-like invariants are much better suited to describe instanton calculations. Respecting the assignments of representations introduced in Table 8.1, we can build the following simplest leading order (in the EFT power counting) invariant

$$\mathcal{I}(C^{(1,8)}_{\rm quqd}) = {\rm Im}\left[e^{-i\theta_{\rm QCD}}\epsilon^{ABC}\epsilon^{abc}\epsilon^{DEF}\epsilon^{def}Y_{{\rm u},Aa}Y_{{\rm u},Bb}C^{(1,8)}_{{\rm quqd},CcDd}Y_{{\rm d},Ee}Y_{{\rm d},Ff}\right], \tag{8.4}$$

which contains the Wilson coefficient $C^{(1,8)}_{{\rm quqd},ijkl}$ and we sum over repeated indices. Note that this exact invariant had already been proposed in App. F of Ref. [103]. In the limit of diagonal Yukawa couplings and vanishing $\theta_{\rm QCD}$ (assumed in Ref. [337]), the SMEFT invariant in Eq. (8.4) has the following form

$$\mathcal{I}(C^{(1,8)}_{\rm quqd}) = 4\left(\prod_{k=1}^{3}\hat{y}_{{\rm u},k}\hat{y}_{{\rm d},k}\right)\sum_{i,j=1}^{3}\frac{{\rm Im}[C^{(1,8)}_{\rm quqd}]_{iijj}}{\hat{y}_{{\rm u},i}\hat{y}_{{\rm d},j}}\,, \tag{8.5}$$

which matches the flavour structure in the instanton computation of the potential shown in Eq. (8.3). The other flavour structure appearing in the instanton computation can be recovered by expanding a second CP-odd determinant-like SMEFT invariant obtained by interchanging the indices C and D of the invariant in Eq. (8.4).

At this point, we would like to understand several points about these new invariants: Why are they more appropriate to describe the flavourful part of instanton computations and how exactly do they arise in those calculations? How can their knowledge help to systematise and simplify those computations? Can a complete basis of the determinant-like invariants be constructed for all SMEFT operators and how are they related to the trace invariants we have previously introduced in Sec. 2.2.3? We will start answering these questions by constructing a complete set of determinant-like invariants for all SMEFT operators next and show explicitly how they arise in instanton computations in Sec. 8.3.

[3] The CKM matrix is assumed to be unity here, which is possible in the SM below the W-boson mass, since all effects of the CKM matrix can be put into effective operators.

8.2.1 A Basis of Determinant-Like Flavour Invariants

In this section, we will show how to construct a complete operator basis of CP-odd flavour invariants of the determinant-like type for all SMEFT operators, suitable for instanton calculations featuring θ_{QCD}, by discussing some explicit examples. By complete, we understand that the flavour invariants capture all sources of CP violation induced in the UV and captured by the SMEFT Wilson coefficients. We do not include *opportunistic* effects where the interference of the real part of a Wilson coefficient with the CKM phase induces CP violation, as previously considered in Ref. [104], i.e. we assume $J_4 = 0$ in the following or at least that these contributions are subleading. Note also, that we only work at the leading order in the EFT, i.e. all flavour invariants will be linear in dimension-6 Wilson coefficients. Higher order effects of multiple insertion of dimension-6 operators or higher dimensional operators are negligible as we estimate in App. 8.A.1.

To test our set for completeness we will use the transfer matrix method presented in Eq. (2.36), which was initially introduced in Ref. [103] to determine the completeness of the sets of CP-odd SMEFT trace invariants. To determine if our set captures all necessary and sufficient conditions for CP violation, we simply compute the rank of the transfer matrix, which has to match the number of phases in the Wilson coefficient which cannot be removed by a field redefinition. Note that, here we do not consider Yukawa matrices with any special values, e.g. degenerate masses, zero masses or texture zeros in the CKM matrix, that enlarge the flavour symmetry of the SM left unbroken by the Yukawa couplings.

$\mathcal{O}_{\text{uH}}$ operator: The first example for building a complete basis with determinant-like invariants we will discuss is the modified Yukawa operator of the up-type quarks, $\mathcal{O}_{\text{uH}} = |H|^2 \bar{Q}\widetilde{H}u$. In order to accommodate for $e^{-i\theta_{\text{QCD}}}$ appearing in the instanton calculations, we have to construct an object that simultaneously removes the $U(1)$ rephasings of the exponentiated θ-angle, while at the same time being invariant under the non-Abelian part of the flavour symmetry and linear in the Wilson coefficient. Following the previous discussion, the simplest combination of Lagrangian parameters fulfilling all these requirements is

$$\text{Im}\left[e^{-i\theta_{\text{QCD}}}\epsilon^{IJK}\epsilon^{ijk}Y_{\text{u},Ii}Y_{\text{u},Jj}C_{\text{uH},Kk}\det Y_{\text{d}}\right], \tag{8.6}$$

where the rephasings of the Yukawa couplings and the Wilson coefficients precisely cancel those of $e^{-i\theta_{\text{QCD}}}$ and the determinant-like structure of the Levi-Civita symbols ensures the invariance under the $SU(3)$ part of the flavour group. Starting from the form in Eq. (8.6), we can now systematically construct flavour invariants that can capture all phases in the Wilson coefficient C_{uH} by using the matrices $X_{\text{u,d}} = Y_{\text{u,d}}Y^{\dagger}_{\text{u,d}}$, transforming in the adjoint of $SU(3)_{\text{Q}}$, to project out different entries of the Wilson coefficients.

Using the transfer matrix method, it can be easily verified that a set of flavour invariants capturing all sources of CP violation in the Wilson coefficient of the operator $\mathcal{O}_{\text{uH}}$, for $J_4 = J_\theta = 0$, is

$$\begin{gathered}\mathcal{I}_{0000}(C_{\text{uH}}),\, \mathcal{I}_{1000}(C_{\text{uH}}),\, \mathcal{I}_{0100}(C_{\text{uH}}),\, \mathcal{I}_{1100}(C_{\text{uH}}),\, \mathcal{I}_{0110}(C_{\text{uH}}),\\ \mathcal{I}_{2200}(C_{\text{uH}}),\, \mathcal{I}_{0220}(C_{\text{uH}}),\, \mathcal{I}_{1220}(C_{\text{uH}}),\, \mathcal{I}_{0122}(C_{\text{uH}})\,,\end{gathered} \tag{8.7}$$

where we have defined

$$\mathcal{I}_{abcd}(C_{\rm uH}) \equiv {\rm Im}\left[e^{-i\theta_{\rm QCD}}\epsilon^{IJK}\epsilon^{ijk}Y_{{\rm u},Ii}Y_{{\rm u},Jj}\left(X_{\rm u}^a X_{\rm d}^b X_{\rm u}^c X_{\rm d}^d C_{\rm uH}\right)_{Kk}\det Y_{\rm d}\right]. \tag{8.8}$$

$\mathcal{O}^{(1,8)}_{\rm quqd}$ operators: After completing this rather straightforward example of a bilinear fermion operator that only contains 9 CP-violating parameters, we will return to the 4-fermion operator $\mathcal{O}^{(1)}_{\rm quqd}$, and its $SU(3)$ adjoint form $\mathcal{O}^{(8)}_{\rm quqd}$, that appeared in the introduction. Following similar considerations as for the last operator, a complete invariant basis can be constructed for these operators by defining the following two structures

$$\begin{aligned}
\mathcal{A}^{a_1,b_1,c_1,d_1}_{a_2,b_2,c_2,d_2}(C^{(1,8)}_{\rm quqd}) &= {\rm Im}\Big[e^{-i\theta_{\rm QCD}}\epsilon^{ABC}\epsilon^{abc}\epsilon^{DEF}\epsilon^{def}Y_{{\rm u},Aa}Y_{{\rm u},Bb}\left(X_{\rm u}^{a_1}X_{\rm d}^{b_1}X_{\rm u}^{c_1}X_{\rm d}^{d_1}\right)_C{}^{C'} \\
&\quad\times C^{(1,8)}_{{\rm quqd},C'cD'd}\left(X_{\rm u}^{a_2}X_{\rm d}^{b_2}X_{\rm u}^{c_2}X_{\rm d}^{d_2}\right)_D{}^{D'}Y_{{\rm d},Ee}Y_{{\rm d},Ff}\Big], \\
\mathcal{B}^{a_1,b_1,c_1,d_1}_{a_2,b_2,c_2,d_2}(C^{(1,8)}_{\rm quqd}) &= {\rm Im}\Big[e^{-i\theta_{\rm QCD}}\epsilon^{ABC}\epsilon^{abc}\epsilon^{DEF}\epsilon^{def}Y_{{\rm u},Aa}Y_{{\rm u},Bb}\left(X_{\rm u}^{a_1}X_{\rm d}^{b_1}X_{\rm u}^{c_1}X_{\rm d}^{d_1}\right)_D{}^{C'} \\
&\quad\times C^{(1,8)}_{{\rm quqd},C'cD'd}\left(X_{\rm u}^{a_2}X_{\rm d}^{b_2}X_{\rm u}^{c_2}X_{\rm d}^{d_2}\right)_C{}^{D'}Y_{{\rm d},Ee}Y_{{\rm d},Ff}\Big].
\end{aligned} \tag{8.9}$$

Here, the index assignment $\mathcal{A}^{0000}_{0000}(C^{(1,8)}_{\rm quqd})$ corresponds to the invariant in Eq. (8.4) and $\mathcal{B}^{0000}_{0000}(C^{(1,8)}_{\rm quqd})$ corresponds to the second invariant mentioned in the last section, where the indices C and D are interchanged. The operator $\mathcal{O}^{(1,8)}_{\rm quqd}$ has 81 phases that can interfere with the marginal SM Yukawa couplings. The full set of 81 determinant-like invariants for these operators can be found in Ref. [3].

$\mathcal{O}^{(1,3)}_{\rm lequ}$ operators: Determinant-like flavour invariants can also be built for operators containing lepton fields, like the semi-leptonic operator $\mathcal{O}^{(1)}_{\rm lequ} = \left(\bar{L}e\right)\left(\bar{Q}u\right)$ and its $SU(2)$ adjoint form $\mathcal{O}^{(3)}_{\rm lequ}$. The invariants capturing the 27 CP-odd parameters of their Wilson coefficients $C^{(1,3)}_{\rm lequ}$ have the following form

$$\mathcal{I}^f_{abcd}(C^{(1,3)}_{\rm lequ}) \equiv {\rm Im}\left[e^{-i\theta_{\rm QCD}}\epsilon^{IJK}\epsilon^{ijk}Y_{{\rm u},Ii}Y_{{\rm u},Jj}\left(X_{\rm u}^a X_{\rm d}^b X_{\rm u}^c X_{\rm d}^d\right)_K{}^L\left(Y_{\rm e}^\dagger X_{\rm e}^f\right)^{mN}C^{(1,3)}_{{\rm lequ},NmLk}\det Y_{\rm d}\right]. \tag{8.10}$$

The index assignments for a complete set of CP-odd flavour invariants can be found in Ref. [3].

$\mathcal{O}^{(1,3)}_{\rm Hq}$ operators: As a last example, we will discuss the construction of determinant-like invariants for an operator which is not charged under the $U(1)$ rephasings of the flavour group. One such operator is the hermitian operator $\mathcal{O}^{(1)}_{\rm Hq} = \left(H^\dagger i\overleftrightarrow{D}_\mu H\right)\left(\bar{Q}\gamma^\mu Q\right)$ and its $SU(2)$ adjoint form $\mathcal{O}^{(3)}_{\rm Hq}$, for which the CP-odd parameters in the Wilson coefficients $C^{(1,3)}_{\rm Hq}$ can be written in a flavour-invariant way as follows

$$\mathcal{I}_{1100}(C^{(1,3)}_{\rm Hq}),\ \mathcal{I}_{2200}(C^{(1,3)}_{\rm Hq}),\ \mathcal{I}_{1122}(C^{(1,3)}_{\rm Hq}), \tag{8.11}$$

where we have defined

$$\mathcal{I}_{abcd}(C_{\rm Hq}^{(1,3)}) \equiv {\rm Im}\left[e^{-i\theta_{\rm QCD}}\epsilon^{IJK}\epsilon^{ijk}Y_{{\rm u},Ii}Y_{{\rm u},Jj}\left(X_{\rm u}^a X_{\rm d}^b X_{\rm u}^c X_{\rm d}^d\, C_{\rm Hq}^{(1,3)}\, Y_{\rm u}\right)_{Kk} \det Y_{\rm d}\right]. \tag{8.12}$$

Following this procedure for the remaining flavourful dimension-6 operators in the SMEFT, a complete set of flavour invariants for those operators capturing all their CP-violating effects can be built for all operators in the Warsaw basis [87], that is suitable for non-perturbative computations featuring an exponentiated $\theta_{\rm QCD}$. A full set of flavour invariants for all operators can be found in Ref. [3].

Let us once again emphasise that these new invariants are redundant in the presence of the trace invariants, as those were already a complete basis of invariants which fully characterise the CP-violating phases of the flavourful dimension-6 SMEFT. Hence, there must exist relations, that express the determinant-like invariants in terms of the trace invariants and vice-versa. These relations can be found by index manipulations of the determinant-like invariants and by employing identities of the Levi-Civita symbol. For example, the invariants in Eq. (8.11) can be rewritten as

$$\begin{aligned}\mathcal{I}_{abcd}(C_{\rm Hq}^{(1,3)}) =&{\rm Im}\left[\left(e^{-i\theta_{\rm QCD}}\det\left(Y_{\rm u}Y_{\rm d}\right)\right)\epsilon^{IJK}\epsilon_{IJL}\left(X_{\rm u}^a X_{\rm d}^b X_{\rm u}^c X_{\rm d}^d C_{\rm Hq}^{(1,3)}\right)_K^{\ \ L}\right]\\ =&2\left(J_\theta\, R_{abcd}(C_{\rm Hq}^{(1,3)}) + K_\theta\, L_{abcd}(C_{\rm Hq}^{(1,3)})\right)\,,\end{aligned} \tag{8.13}$$

where $R_{abcd}(C) = {\rm Re}\left[{\rm Tr}\left(X_{\rm u}^a X_{\rm d}^b X_{\rm u}^c X_{\rm d}^d C\right)\right]$ and $L_{abcd}(C) = {\rm Im}\left[{\rm Tr}\left(X_{\rm u}^a X_{\rm d}^b X_{\rm u}^c X_{\rm d}^d C\right)\right]$, as defined in Ref. [103]. There exist similar relations for all other operators, such as

$$\mathcal{I}_{abcd}(C_{\rm uH}) = 2\left(J_\theta\, R_{(a-1)bcd}(C_{\rm uH}Y_{\rm u}^\dagger) + K_\theta\, L_{(a-1)bcd}(C_{\rm uH}Y_{\rm u}^\dagger)\right)\,, \tag{8.14}$$

$$\mathcal{I}_{abcd}^f(C_{\rm lequ}^{(1,3)}) = 2\left(J_\theta\,{\rm Im}\, A_{(a-1)bcd}^f(C_{\rm lequ}^{(1,3)}) + K_\theta\,{\rm Re}\, A_{(a-1)bcd}^f(C_{\rm lequ}^{(1,3)})\right)\,, \tag{8.15}$$

where $A_{abcd}^f(C_{\rm lequ}^{(1,3)}) = X_{{\rm e},ji}^f\left(X_{\rm u}^a X_{\rm d}^b X_{\rm u}^c X_{\rm d}^d\right)_{lk} Y_{{\rm e},mj}^\dagger Y_{{\rm u},nl} C_{{\rm lequ},imkn}^{(1,3)}$. This procedure allows us to map all determinant-like invariants directly to the trace invariants of Ref. [103] for all operators up to the invariants of the form $\mathcal{I}_{0bcd}(C_{\rm uH})$, where inverse Yukawa couplings appear in the trace invariants (c.f. $\mathcal{I}_{0000}(C_{\rm uH})$ in Eq. (8.14)). We refer to Ref. [3], for a discussion on how these latter invariants featuring powers of inverse Yukawas can also be mapped to the old trace basis of Ref. [103]. The relations also make apparent, that the determinant-like invariants capture both the CP violation due to the phases induced by SMEFT operators and the one due to the interference between the CP-even parts of the SMEFT operators with the SM strong CP phase.

8.3 The Interplay of Topological Susceptibilities and Flavour Invariants

Before jumping into the instanton computations, we will first clarify how new sources of CP violation can contribute to the axion potential. In particularm, we want to compute how the

CP-violating SMEFT operators

$$\mathcal{L} \supset \frac{C_{\mathcal{O}}^{ij\cdots}}{\Lambda_{\not{CP}}^{D-4}} \mathcal{O}^{D,ij\cdots} \,, \tag{8.16}$$

can offset the minimum of the axion potential in the presence of small instantons, where D is the mass dimension of the EFT operator $\mathcal{O}$ and $i, j, \ldots$ are its flavour indices. In the following, we will focus on the dimension-6 SMEFT operators only and will justify in App. 8.A.1 why they give the leading contribution. Because we only consider *CP-odd* SMEFT operators, the operators can only contribute linearly to the part of the θ-dependent vacuum energy linear in θ [357]

$$V(\bar\theta, C_{\mathcal{O}}) = \frac{1}{2}\left(u_\theta\,\bar\theta^{\,2} + 2u_{\theta\mathcal{O}}\,\bar\theta\, C_{\mathcal{O}} + u_{\mathcal{O}}\, C_{\mathcal{O}}^2\right) , \tag{8.17}$$

where the objects $u_\theta, u_{\theta\mathcal{O}}, u_{\mathcal{O}}$ can be computed in terms of SM and SMEFT operators. After making θ dynamical by adding an axion to the theory, we can understand Eq. (8.17) as the effective potential of the axion after integrating out all of the SM fields. Then, $u_\theta, u_{\theta\mathcal{O}}, u_{\mathcal{O}}$ can be obtained by performing a matching computation for the effective action of the terms up to quadratic order in θ and the SMEFT operator $\mathcal{O}$

$$u_\theta \sim \left\langle (G\tilde G)^2 \right\rangle, \qquad u_{\theta\mathcal{O}} \sim \frac{1}{\Lambda_{\not{CP}}^{D-4}} \left\langle G\tilde G\,\mathcal{O}\right\rangle, \qquad u_{\mathcal{O}} \sim \frac{1}{\Lambda_{\not{CP}}^{2D-8}} \left\langle \mathcal{O}^2 \right\rangle \,. \tag{8.18}$$

As such, the $u_{\mathcal{O}}$ term can be neglected compared to the other two terms. Note that Eq. (8.17) introduces a linear term in $\bar\theta$, which if non-zero shifts the minimum of the vacuum energy. By explicitly promoting θ to the dynamical axion field a/f_a, the induced value of $\bar\theta \equiv \langle a/f_a\rangle$ is determined by Eq. (8.17). To be concrete, the potential can be re-written in terms of the axion field a

$$V(a) = \chi_{\mathcal{O}}(0)\frac{a}{f_a} + \frac{1}{2}\chi(0)\left(\frac{a}{f_a}\right)^2 \,, \tag{8.19}$$

where we have introduced $\chi(0)$ and $\chi_{\mathcal{O}}(0)$ to replace u_θ and $u_{\theta\mathcal{O}}$, respectively, which is defined as [44, 169, 358, 359]

$$\chi(0) = -i \lim_{k\to 0} \int d^4x\, e^{ikx} \left\langle 0 \middle| T\left\{ \frac{g^2}{32\pi^2} G\tilde G(x)\,,\, \frac{g^2}{32\pi^2} G\tilde G(0)\right\} \middle| 0 \right\rangle , \tag{8.20}$$

known as the QCD topological susceptibility and

$$\chi_{\mathcal{O}}(0) = -i \lim_{k\to 0} \int d^4x\, e^{ikx} \left\langle 0 \middle| T\left\{ \frac{g^2}{32\pi^2} G^a_{\mu\nu}\tilde G_a^{\mu\nu}(x)\,,\, \frac{C_{\mathcal{O}}^{ij\cdots}}{\Lambda_{\not{CP}}^{D-4}} \mathcal{O}^{D,ij\cdots}(0)\right\} \middle| 0 \right\rangle . \tag{8.21}$$

Minimising the potential in Eq. (8.19), yields the following expression for the shift of the minimum in the axion potential

$$\theta_{\rm ind} \equiv -\frac{\chi_{\mathcal{O}}(0)}{\chi(0)} \,. \tag{8.22}$$

Experimental bounds on the neutron EDM lead to the constraint $\theta_{\text{ind}} \lesssim 10^{-10}$, which can be used to obtain limits on any UV parameters contained in $\chi_{\mathcal{O}}(0)$.

Usually, models of axions or axion-like particles (ALPs) are constructed with a $U(1)$ Peccei–Quinn symmetry in mind, which dictates the ALP couplings to the SM particles – either directly or in an EFT after integrating out the heavy modes from the theory. If one allows for some explicit breaking of the $U(1)$ symmetry[4] responsible for the Nambu–Goldstone boson nature of the ALP, an axion potential can be generated in ordinary perturbation theory. The interactions of the ALP with the SM particles, including those breaking the shift symmetry, can be captured in an EFT in a relatively model-independent way. In this case, the axion potential can be determined by calculating the Coleman–Weinberg potential in the ALP EFT including operators that break the shift symmetry of the ALP explicitly. The tadpole term of the resulting potential should be proportional to the invariants presented in Chap. 6, that capture all sources of shift symmetry breaking at the leading order in the effective theory (see also Ref. [273]).

8.3.1 Topological Susceptibilities

In this section, we will clarify how to compute the correlators appearing as the coefficients in the axion potential in Eq. (8.19) in the instanton background from the path integral. In particular, we will summarise the main points introduced in Sec. 2.6 that are relevant for the computation in the instanton background following the computations of Ref. [143].

To illustrate the different steps in evaluating the correlator with an insertion of an effective operator defined in Eq. (8.21), we consider a generic dimension-six operator $\mathcal{O}[\varphi_{\text{I}}, \varphi]$, where φ_{I} are fields whose zero modes take on a special form in the instanton background (e.g. gluon and quark fields), and φ denotes the other fields unrelated to instanton dynamics (e.g. Higgs or lepton fields). The correlator associated with $\mathcal{O}$ is given by

$$\begin{aligned}\chi_{\mathcal{O}}(0) &= -i \lim_{k\to 0} \int d^4x\, e^{ikx} \left\langle 0 \left| T\left\{ \frac{g^2}{32\pi^2} G\tilde{G}(x)\, , \frac{C_{\mathcal{O}}}{\Lambda^2_{\cancel{CP}}} \mathcal{O}[\varphi_{\text{I}}, \varphi](0) \right\} \right| 0 \right\rangle \\ &= e^{-i\theta_{\text{QCD}}} \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho) \int \prod_{f=1}^{N_f} \left(\rho\, d\xi_f^{(0)} d\bar{\xi}_f^{(0)}\right) \\ &\times \int \mathcal{D}\varphi\, e^{-S_0[\varphi] - S_{\text{int}}[\varphi_{\text{I}}, \varphi]} \int d^4x \frac{g^2}{32\pi^2} G\tilde{G}(x) \frac{C_{\mathcal{O}}}{\Lambda^2_{\cancel{CP}}} \mathcal{O}[\varphi_{\text{I}}, \varphi](0) \Big|_{\text{1-(a.-)inst.}} ,\end{aligned} \tag{8.23}$$

where $S_0[\varphi]$ is the free Euclidean action of the fields φ independent of the instanton dynamics and $S_{\text{int}}[\varphi_{\text{I}}, \varphi]$ is the interacting actions between the fields φ_{I} and φ. The correlators are evaluated by performing perturbation theory with the non-zero modes around the semi-classical instanton background field given by the explicit expression of the zero modes in the instanton background. Due to the explicit form of the zero modes, the instanton computations simplify drastically. We summarise the essential steps of the computations as follows

[4] Even if this explicit breaking is not introduced by hand it will be generated by quantum gravity effects as discussed earlier in the context of the axion quality problem.

- *Fields with instanton solutions* $\varphi_{\rm I}$*:* The field $\varphi_{\rm I}$ is expanded in eigenmodes, where the zero modes of $\varphi_{\rm I}$ take on the form dictated by the BPST instanton solution constructed in Sec. 2.6. Most importantly, the fermion fields are expanded as

$$\psi_f(x) = \sum_k \xi_f^{(k)} \psi^{(k)}\,, \qquad \bar{\psi}_f(x) = \sum_k \bar{\xi}_f^{(k)} \bar{\psi}^{(k)}\,, \tag{8.24}$$

  where $\xi_f^{(k)}$, $\bar{\xi}_f^{(k)}$ are Grassmann variables, f is a fermion flavour index and the explicit form of $\psi^{(0)}$ is given in Eq. (2.144). Following the discussion in Ref. [143], in all explicit computations that follow, we will expand the interacting action between the zero modes and non-zero modes to zeroth order. This will allow us to integrate out the non-zero modes of $\varphi_{\rm I}$ from the path integral. The path integral over the zero modes reduces to the integration over collective coordinates as introduced in Sec. 2.6. Thus, we can directly replace the path integral of $\varphi_{\rm I}$ using 't Hooft's result [143]

$$\int \mathcal{D}\varphi_{\rm I}\, e^{-S_E[\varphi_{\rm I}]} \to e^{-i\theta_{\rm QCD}} \int d^4 x_0 \int \frac{d\rho}{\rho^5} d_N(\rho) \int \prod_{f=1}^{N_f} \left(\rho\, d\xi_f^{(0)} d\bar{\xi}_f^{(0)}\right), \tag{8.25}$$

  where in particular the integration over the fermion fields in the path integral reduces to a simple Grassmann integration with $d\xi^{(0)}$, $d\bar{\xi}^{(0)}$ the Grassmann integration measure and $d_N(\rho)$ is the instanton density in the $SU(N)$ theory (see Eq. (2.150)) with ρ denoting the instanton size.

- *Fields without instanton solutions* φ*:* The remaining fields φ, are treated like in ordinary perturbation theory. After expanding the exponential of the interacting action $e^{-S_{\rm int}[\varphi_{\rm I},\varphi]}$[5], one can compute the non-vanishing contributions to the correlation function by contracting the fields φ appearing in the correlators to propagators by evaluating the path integral with the exponentiated free action (c.f. Eq. (2.122)). Diagrammatically, this can be understood as closing the remaining field lines of the fields φ not related to the instanton dynamics in the interaction vertices with the fields $\varphi_{\rm I}$ directly coupled to the instanton vertex, see e.g. Fig. 8.1a.

- In a last step, the zero mode profiles of $\varphi_{\rm I}$ given by Eqs. (2.129) and (2.144) are substituted into the expression and the remaining loop integrals due to φ and collective coordinate integrals due to $\varphi_{\rm I}$ are evaluated. Most of these calculations are carried out in App. 8.A. Finally, the integral over instanton size ρ is performed in Sec. 8.4, for which a specific UV completion responsible for the instanton dynamics has to be specified.

The other correlation function appearing in Eq. (8.19) is (to the accuracy we work in the SMEFT) the QCD topological susceptibility defined in Eq. (8.20). This two-point correlation

[5]There are two different contributions. The first one is due to the Grassmann variables of the zero modes, which are simply expanded to the non-vanishing order dictated by the Grassmann nature of these variables and the Grassmann integration. The second type of contribution are those where the interacting action only features fields which do not take part in the instanton dynamics, as we will see in the computation of the semi-leptonic operator in Sec. 8.3.4.

function has been computed in the literature, assuming that $\chi(0)$ only receives contributions from the SM. Within the perturbative regime and in the 1-instanton approximation it is given by [20, 239]

$$\chi(0) = -3!\,(2K_\theta)\; i \int \frac{d\rho}{\rho^5} d_N(\rho) \frac{1}{(6\pi^2)^3}\,, \tag{8.26}$$

where $K_\theta = \mathrm{Re}\left[e^{-i\theta_{\mathrm{QCD}}} \det\left(Y_{\mathrm{u}} Y_{\mathrm{d}}\right)\right]$ as introduced in footnote 2.

8.3.2 Relevance of Determinant-Like Flavour Invariants

Before we show all of the details of the instanton computations, we want to put the focus on how the determinant-like flavour structures, that we previously claimed would appear, arise in the computations. The essential point that allows us to understand the appearance of the invariants is the treatment of the fermionic contributions in the instanton background. In particular, as we just learned, the fermion fields are expanded in their eigenmodes, such that the path integral over the zero modes, which obtain a specific functional form in the instanton background, reduce to a simple Grassmannian integral. Due to the rules of Grassmann calculus,

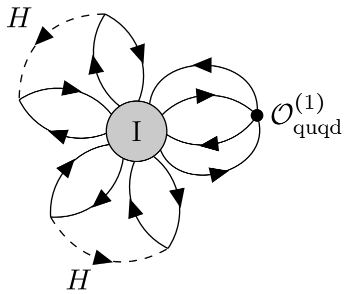
$$\int d\xi\; \xi = 1\,, \qquad \int d\xi\; 1 = 0,, \qquad \xi^2 = 0\,, \tag{8.27}$$

for a single Grassmann variable ξ, only some terms of the exponentiated interacting action will survive. Furthermore, the different terms in the power expansion of the exponential will come with different signs due to the anti-commutation property of Grassmann variables $\{\xi_1, \xi_2\} = 0$ for two Grassmann variables $\xi_{1,2}$. Using these facts, it is straightforward to prove that the following Grassmann integration identities hold true

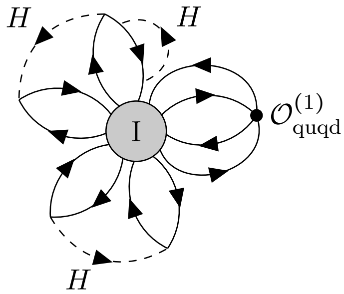
$$\begin{aligned}
\int d^3\xi_1 d^3\xi_2\; e^{\xi_1 A \xi_2} &= \det A\,,\\
\int d^3\xi_1 d^3\xi_2\; e^{\xi_1 A \xi_2}\xi_1 B \xi_2 &= \frac{1}{2}\epsilon^{i_1 i_2 i_3}\epsilon^{j_1 j_2 j_3} A_{i_1 j_1} A_{i_2 j_2} B_{i_3 j_3}\,,\\
\int d^3\xi_1 d^3\xi_2 d^3\xi_3 d^3\xi_4\; e^{\xi_1 A \xi_2 + \xi_3 B \xi_4}\xi_1 C \xi_2 &= \frac{1}{2}\epsilon^{i_1 i_2 i_3}\epsilon^{j_1 j_2 j_3} A_{i_1 j_1} A_{i_2 j_2} C_{i_3 j_3} \det B\,,\\
\int d^3\xi_1 d^3\xi_2 d^3\xi_3 d^3\xi_4\; e^{\xi_1 A \xi_2 + \xi_3 B \xi_4}\xi_1 C \xi_2\, \xi_3 D \xi_4 &= \frac{1}{4}\epsilon^{i_1 i_2 i_3}\epsilon^{j_1 j_2 j_3} A_{i_1 j_1} A_{i_2 j_2} C_{i_3 j_3}\\
&\quad \times \epsilon^{k_1 k_2 k_3}\epsilon^{l_1 l_2 l_3} B_{k_1 l_1} B_{k_2 l_2} D_{k_3 l_3}\,,
\end{aligned} \tag{8.28}$$

where $\xi_{1,\ldots,4}$ are three-dimensional Grassmann variables and A, B, C, D are 3×3 matrices. These identities are at the origin of the appearance of flavourful objects contracted with Levi-Civita symbols in the calculation, which we refer to as determinant-like.

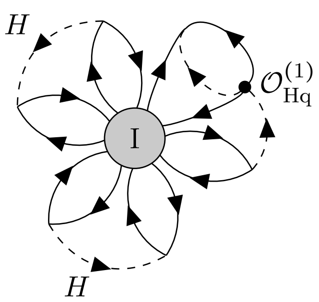
As such, in computations where the CP-odd SMEFT operator inserted in a correlator contains quark zero modes, which are integrated over in the Grassmann integration, the determinant-like invariants introduced in Sec. 8.2.1 are better suited at describing effects of CP violation. This is because, as we will show in all details below, in the computation of the correlator these invariants will arise naturally and in contrast to the trace basis of CP-odd invariants, no further relations have to be used to fully express the final result in terms of the CP-odd SMEFT invariants and the SM flavour invariants shown in Eq. (2.98).



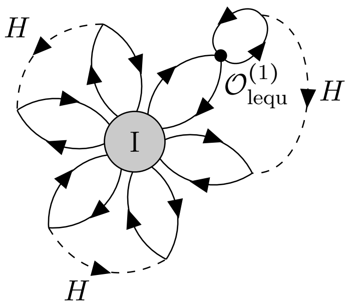
(a) Instanton diagram with an insertion of the effective operator $\mathcal{O}^{(1)}_{\rm ququd}$.



(b) Instanton diagram with an insertion of the effective operator $\mathcal{O}^{(1)}_{\rm ququd}$ and additional Yukawa coupling insertions, corresponding to invariants of higher order in the Yukawa couplings.



(c) Instanton diagram with an insertion of a non-chirality-flipping effective operator $\mathcal{O}^{(1)}_{\rm Hq}$.



(d) Instanton diagram with an insertion of an effective operator, giving rise to mixed trace and determinant-like invariants. One example is the insertion of the effective operator $\mathcal{O}^{(1)}_{\rm lequ}$.

Figure 8.1: Examples of instanton diagrams corresponding to invariants discussed in the text. Here, the grey blob depicts the instanton background that the fermions (solid lines) are coupled to. The fermion lines are closed via Yukawa interactions with the Higgs (dashed lines).

Furthermore, a direct relation between diagrammatic contributions and invariants is evident. Consider the example of the calculation performed in Ref. [337], where the correlator from an insertion of the effective operator $\mathcal{O}^{(1)}_{\rm ququd}$ was studied. Diagrammatically this process can be understood as that of Fig. 8.1a. In the diagram, one can observe that all fermion legs of the effective operator are connected to the instanton background and hence, all the fermions in the effective operator will simply be the zero modes, which take on the special form shown in Eq. (2.144) in the instanton background. Therefore, whenever a fermion line is directly connected to the instanton background, the indices of those fermions will be contracted in a determinant-like manner in the flavour structure of the resulting contribution. Indeed, as we will prove explicitly in the next section, the diagram in Fig. 8.1a gives a contribution proportional to the introduced invariants $\mathcal{A}^{0000}_{0000}(C^{(1)}_{\rm ququd})$ and $\mathcal{B}^{0000}_{0000}(C^{(1)}_{\rm ququd})$.

Another interesting contribution which illustrates the previous points is the contribution from the insertion of the operator $\mathcal{O}^{(1)}_{\rm lequ}$. The corresponding diagram is that of Fig. 8.1d and only the quarks emerging from the effective operator have zero modes, as the leptons are not charged under the $SU(3)_c$ gauge group responsible for the instanton dynamics. Indeed, looking at the leading invariant $I^f_{0000}(C^{(1)}_{\rm lequ})$, we see exactly that only the quark indices are contracted with the anti-symmetric ϵ-structure, whereas the lepton indices are contracted in a trace-like manner over a matrix product with a lepton Yukawa coupling.

A final illustrative example is that of rephasing invariant operators such as $\mathcal{O}^{(1)}_{\rm Hq}$. In this case, even at the lowest order in Yukawa couplings, one cannot build an invariant where both quark indices are directly contracted with an ϵ-structure; at most one index is contracted, as shown in the invariant $\mathcal{I}_{abcd}(C^{(1)}_{\rm Hq})$. Diagrammatically, this means that only one of the fermion lines is directly connected to the instanton background and only one of the fermions in the effective operator can be a zero mode. This case is illustrated in Fig. 8.1c.

These examples have given us an intuitive understanding of why and how the determinant-like invariants (and no extra flavour structures) appear in the instanton computations. Next, we will show how these patterns arise explicitly, after which we will generalise our examples to generic selection rules on all CP-odd SMEFT operators guided by the flavour invariants.

8.3.3 Four-Quark Operator

Usually, in instanton computations the open fermion legs coupled directly to the background are closed by the use of mass terms or Yukawa couplings, each giving a different scaling of the integrand with the instanton size ρ [240]. In the presence of effective fermionic operators, they can also be used to contract some of the open fermion legs.

We will make use of this in the first example we want to explicitly discuss, the operator $\mathcal{O}^{(1)}_{\rm ququd}$, which can give rise to the instanton diagram in Fig. 8.1a. Since we only consider $SU(3)_c$ instantons here, the SM $SU(2)$ gauge group is unrelated to the instanton dynamics and the $SU(2)$ indices of the quarks can be treated in the same way as a flavour index. As for the flavour indices, the explicit form of the zero mode will therefore also not depend on the $SU(2)$ index, which is just another label for the Grassmann variable in the expansion of the fermion fields in their eigenmodes. The correlator, Eq. (8.21), induced by the 4-fermion operator can be calculated as[6]

$$\begin{aligned}
\chi^{(1)}_{\rm ququd}(0)^{\rm 1-inst.} &= -i\lim_{k\to 0}\int d^4x\, e^{ikx}\left\langle 0\left|T\left\{\frac{1}{32\pi^2}G\widetilde{G}(x), \frac{C^{(1)}_{\rm ququd}}{\Lambda^2_{\not{CP}}}\mathcal{O}^{(1)}_{\rm ququd}(0)\right\}\right|0\right\rangle ,\\
&= e^{-i\theta_{\rm QCD}}\int d^4x_0\int\frac{d\rho}{\rho^5}d_N(\rho)\int\mathcal{D}H\mathcal{D}H^\dagger\, e^{-S_0[H,H^\dagger]}\int\prod_{f=1}^{3}\left(\rho^2\, d\xi^{(0)}_{u_f}d\xi^{(0)}_{d_f}d^2\bar{\xi}^{(0)}_{Q_f}\right) \qquad (8.29)\\
&\times e^{\int d^4x(\bar{Q}Y_{\rm u}\widetilde{H}u+\bar{Q}Y_{\rm d}Hd+{\rm h.c.})(x)}\frac{1}{32\pi^2}\int d^4x\, G\widetilde{G}(x)\left(\frac{C^{(1)}_{\rm ququd}}{\Lambda^2_{\not{CP}}}\bar{Q}u\bar{Q}d(0)+{\rm h.c.}\right),
\end{aligned}$$

where $d^2\bar{\xi}^{(0)}_{Q_f}\equiv d\bar{\xi}^{(0)}_{Q^1_f}\,d\bar{\xi}^{(0)}_{Q^2_f}$ for the two components of the $SU(2)$ quark doublet. Here, we have already performed all of the steps described in Sec. 2.6 up to the expansion of the exponential

[6] Note, that all computations are done in Euclidean space by Wick-rotating the time coordinate everywhere in the calculations.

of the action and the Grassmann integration. In the 1-instanton background with topological charge $Q = +1$ only the zero modes of the right-handed fermions $u, d, Q^\dagger$ have the particular functional form of Eq. (2.144), while the other chirality is vanishing and will instead contribute in the anti-instanton scenario.

The next step is to expand the exponential of the interacting action of the fermions and Higgs, such that precisely enough fermion fields appear in the Grassmann integral to obtain a non-vanishing result. We will also make the $SU(2)$ indices of all $SU(2)$ doublets explicit in the following calculations by giving all $SU(2)$ doublets upper case indices. We find

$$\begin{aligned}
\chi^{(1)}_{\text{quqd}}(0)^{1-\text{inst.}} &= e^{-i\theta_{\text{QCD}}} \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho) \int \mathcal{D}H\mathcal{D}H^\dagger\, e^{-S_0[H,H^\dagger]} \prod_{f=1}^{3} \left(\rho^2\, d\xi^{(0)}_{u_f} d\xi^{(0)}_{d_f} d^2\bar{\xi}^{(0)}_{Q_f}\right) \\
&\times \int d^4x_1 d^4x_2 d^4x_3 d^4x_4\, \frac{1}{4!} \Bigg[\sum_{\substack{\text{perm. over}\\ \text{fermion fields}}} \bar{\xi}^{(0)}_{Q^I_{i_1}} (\bar{\psi}^{(0)} Y_{\text{u},i_1j_1} \widetilde{H}^I P_R \psi^{(0)})(x_1) \xi^{(0)}_{u_{j_1}} \\
&\times \bar{\xi}^{(0)}_{Q^J_{i_2}} (\bar{\psi}^{(0)} Y_{\text{u},i_2j_2} \widetilde{H}^J P_R \psi^{(0)})(x_2) \xi^{(0)}_{u_{j_2}} \quad \bar{\xi}^{(0)}_{Q^K_{k_1}} (\bar{\psi}^{(0)} Y_{\text{d},k_1l_1} H^K P_R \psi^{(0)})(x_3) \xi^{(0)}_{d_{l_1}} \\
&\times \bar{\xi}^{(0)}_{Q^L_{k_2}} (\bar{\psi}^{(0)} Y_{\text{d},k_2l_2} H^L P_R \psi^{(0)})(x_4) \xi^{(0)}_{d_{l_2}} \int d^4x \frac{G\widetilde{G}(x)}{32\pi^2} \Bigg(\frac{C^{(1)}_{\text{quqd},mnop}}{\Lambda^2_{\not{CP}}} \bar{\xi}^{(0)}_{Q^M_m} (\bar{\psi}^{(0)} P_R \psi^{(0)}) \xi^{(0)}_{u_n}\, \epsilon_{MN} \\
&\times \bar{\xi}^{(0)}_{Q^N_o} (\bar{\psi}^{(0)} P_R \psi^{(0)}) \xi^{(0)}_{d_p} \Bigg)(0) \Bigg],
\end{aligned} \tag{8.30}$$

where the indices m, M of $\xi^{(0)}_{Q^M_m}$ denote the flavour and $SU(2)$ indices, respectively, of the zero mode Grassmann vector ξ_Q, which in this case is six-dimensional. In the next step, we essentially rederive the identities shown in Eq. (8.28) by integrating over all Grassmann variables of the zero modes and considering all the permutations over the fermion fields appearing after expanding the exponential. Then, as expected, we find that the Levi-Civita structures appear explicitly

$$\begin{aligned}
\chi^{(1)}_{\text{quqd}}(0)^{1-\text{inst.}} &= \frac{1}{4\Lambda^2_{\not{CP}}} \Big[e^{-i\theta_{\text{QCD}}} \epsilon^{i_1i_2m} \epsilon^{j_1j_2n} Y_{\text{u},i_1j_1} Y_{\text{u},i_2j_2} C^{(1)}_{\text{quqd},mnop} \epsilon^{k_1k_2o} \epsilon^{l_1l_2p} Y_{\text{d},k_1l_1} Y_{\text{d},k_2l_2} \\
&+ e^{-i\theta_{\text{QCD}}} \epsilon^{i_1i_2m} \epsilon^{j_1j_2n} Y_{\text{u},i_1j_1} Y_{\text{u},i_2j_2} C^{(1)}_{\text{quqd},onmp} \epsilon^{k_1k_2o} \epsilon^{l_1l_2p} Y_{\text{d},k_1l_1} Y_{\text{d},k_2l_2} \Big] \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho) \rho^6 \\
&\times \underbrace{\int \mathcal{D}H\mathcal{D}H^\dagger\, e^{-S_0[H,H^\dagger]} \Big[\int d^4x_1 d^4x_2 (\bar{\psi}^{(0)} H^\dagger_I \epsilon^{IJ} P_R \psi^{(0)})(x_1)\, (\bar{\psi}^{(0)} \epsilon_{JK} H^K P_R \psi^{(0)})(x_2) \Big]^2}_{= 2! \left[\int d^4x_1 d^4x_2 (\bar{\psi}^{(0)} P_R \psi^{(0)})(x_1) \Delta_H(x_1 - x_2) \epsilon_{IJ} \epsilon^{JI} (\bar{\psi}^{(0)} P_R \psi^{(0)})(x_2)\right]^2 \equiv 2!\, \mathcal{I}^2} \\
&\times \left(\epsilon_{MN} \epsilon^{MN} \bar{\psi}^{(0)} P_R \psi^{(0)}\, \bar{\psi}^{(0)} P_R \psi^{(0)} \right)(0) \int d^4x \frac{G\widetilde{G}(x)}{32\pi^2}.
\end{aligned} \tag{8.31}$$

The factor of 1/4 at the beginning of Eq. (8.31) appears because the integral over the fermion zero modes is expressed in terms of the Levi-Civita symbols (see also Eq. (8.28)). The last step is to integrate over the Higgs field in the Euclidean path integral. This can be achieved employing the definition of the Higgs propagator in position space

$$\int \mathcal{D}H\mathcal{D}H^\dagger e^{-S_0[H,H^\dagger]} H_I(x_1) H_J^\dagger(x_2) = \Delta_H(x_1 - x_2)\,\delta_{IJ}\,, \tag{8.32}$$

after which we are left with the integral

$$\mathcal{I} = 2\int d^4x_1 d^4x_2 (\bar{\psi}^{(0)} P_R \psi^{(0)})(x_1) \Delta_H(x_1 - x_2) (\bar{\psi}^{(0)} P_R \psi^{(0)})(x_2)\,, \tag{8.33}$$

multiplying the invariant structure that we set out to find. After some simplifications, we finally arrive at

$$\chi^{(1)}_{\text{quqd}}(0)^{\text{1-inst.}} = \frac{A^{(1)}_{\text{quqd}} + B^{(1)}_{\text{quqd}}}{\Lambda^2_{\not{CP}}} \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho)\rho^6 \mathcal{I}^2 \left(\bar{\psi}^{(0)} P_R \psi^{(0)} \bar{\psi}^{(0)} P_R \psi^{(0)}\right)(0)\,, \tag{8.34}$$

where we have defined

$$\begin{aligned} A^{(1)}_{\text{quqd}} &= e^{-i\theta_{\text{QCD}}} \epsilon^{i_1 i_2 m} \epsilon^{j_1 j_2 n} Y_{\text{u},i_1 j_1} Y_{\text{u},i_2 j_2} C^{(1)}_{\text{quqd},mnop} \epsilon^{k_1 k_2 o} \epsilon^{l_1 l_2 p} Y_{\text{d},k_1 l_1} Y_{\text{d},k_2 l_2}\,, \\ B^{(1)}_{\text{quqd}} &= e^{-i\theta_{\text{QCD}}} \epsilon^{i_1 i_2 m} \epsilon^{j_1 j_2 n} Y_{\text{u},i_1 j_1} Y_{\text{u},i_2 j_2} C^{(1)}_{\text{quqd},onmp} \epsilon^{k_1 k_2 o} \epsilon^{l_1 l_2 p} Y_{\text{d},k_1 l_1} Y_{\text{d},k_2 l_2}\,. \end{aligned} \tag{8.35}$$

The same calculation can be performed with the anti-instanton solution. In this case, the non-vanishing contributions will arise from the Hermitian conjugate terms in the calculation. Furthermore, the winding number $\int d^4x\, G\widetilde{G}(x)$ will flip its sign, which also induces a sign flip in the exponential of θ_{QCD} and due to the anti-self-dual property (c.f. Eq. (2.134)) of the anti-instanton solution, the $G\tilde{G}$ term in the correlator will also flip its sign, giving the total contribution an overall negative sign. After summing up the instanton and anti-instanton contributions, the full result for the correlator induced by $\mathcal{O}^{(1)}_{\text{quqd}}$ reads

$$\begin{aligned} \chi^{(1)}_{\text{quqd}}(0) &= \chi^{(1)}_{\text{quqd}}(0)\big|_{\text{1-inst.}} + \chi^{(1)}_{\text{quqd}}(0)\big|_{\text{1-a.-inst.}} \\ &= \frac{1}{\Lambda^2_{\not{CP}}} \left(A^{(1)}_{\text{quqd}} + B^{(1)}_{\text{quqd}}\right) \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho)\rho^6 \mathcal{I}^2 \left(\bar{\psi}^{(0)} P_R \psi^{(0)}\, \bar{\psi}^{(0)} P_R \psi^{(0)}\right)(0)\Big|_{\text{1-inst.}} \\ &- \frac{1}{\Lambda^2_{\not{CP}}} \left(A^{(1)}_{\text{quqd}} + B^{(1)}_{\text{quqd}}\right)^* \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho)\rho^6 \mathcal{I}^2 \left(\bar{\psi}^{(0)} P_L \psi^{(0)}\, \bar{\psi}^{(0)} P_L \psi^{(0)}\right)(0)\Big|_{\text{1-a.-inst.}}\,. \end{aligned} \tag{8.36}$$

Substituting the explicit form of the fermion zero modes from Eq. (2.144) gives

$$\bar{\psi}_i^{(0)} P_R \psi_i^{(0)} \bar{\psi}_j^{(0)} P_R \psi_j^{(0)}\Big|_{\text{1-inst.}} = \frac{4\rho^4}{\pi^4} \frac{1}{(x_0^2 + \rho^2)^6} = \bar{\psi}_i^{(0)} P_L \psi_i^{(0)} \bar{\psi}_j^{(0)} P_L \psi_j^{(0)}\Big|_{\text{1-a.-inst.}}\,, \tag{8.37}$$

which in turn leads to the result

$$\chi^{(1)}_{\text{ququd}}(0) = \frac{2i}{\Lambda^2_{\not{CP}}} \,\text{Im}\left(A^{(1)}_{\text{ququd}} + B^{(1)}_{\text{ququd}}\right) \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho)\rho^6 \mathcal{I}^2 \left[\frac{4\rho^4}{\pi^4}\frac{1}{(x_0^2+\rho^2)^6}\right] . \tag{8.38}$$

As expected, the final result depends explicitly on the determinant-like CP-odd invariants introduced in Eq. (8.9)

$$\text{Im}(A^{(1)}_{\text{ququd}}) = \mathcal{A}^{0000}_{0000}\left(C^{(1)}_{\text{ququd}}\right) , \quad \text{Im}(B^{(1)}_{\text{ququd}}) = \mathcal{B}^{0000}_{0000}\left(C^{(1)}_{\text{ququd}}\right) . \tag{8.39}$$

We can perform an NDA estimate following Ref. [242] to compare how closely it approximates the full results. The NDA results state the loop factor suppression, $(4\pi)^{-\alpha}$ is given by

$$\alpha = z - 2v + 2p , \tag{8.40}$$

where z is the number of fermion zero modes, v the number of vertices and p the number of propagators in the instanton calculation. The diagram in Fig. 8.1a allows us to read off all the required quantities and we find $\alpha = 12 - 10 + 4 = 6$ for the insertion of $\mathcal{O}^{(1)}_{\text{ququd}}$. After plugging in the explicit form of the zero modes, our final result in Eq. (8.68) has a suppression of $1/(45\pi^6)$. While the powers of π are correctly predicted by the NDA, the numerical factor differs significantly. The difference arises because the computations here have been performed in the unbroken EW phase, whereas the NDA predictions where made without the $SU(2)$ structure. Furthermore, there are some small combinatoric factors which the NDA estimate cannot take into account. Taking all of this into account, the estimate of the NDA predicts a suppression factor of $1/(256\pi^6)$ in Eq. (8.68), which is within one order of magnitude compared to the full calculation.

8.3.4 Semileptonic Four-Fermion Operator

In Sec. 8.2.1, we showed that the semi-leptonic operator $\mathcal{O}^{(1)}_{\text{lequ}}$ can also furnish invariants featuring θ_{QCD}, raising the expectation that the operator can also give a non-vanishing contribution to the axion potential in an instanton background. As the leptons are neutral under $SU(3)_c$ responsible for the instantons, they are not coupled to the instanton vertex directly. Instead, they should be treated as in ordinary perturbation theory like the Higgs field in the last section, which will have consequences for the invariant structure of the lepton couplings in the computation, as we will see now. We will compute the correlator with an insertion of the operator $\mathcal{O}^{(1)}_{\text{lequ}}$, where this time the leptons are kept in the path integral compared to the previous computation. As before, we will split off the quark zero modes and integrate over the non-zero modes of the fields. This yields

$$\begin{aligned}\chi^{(1)}_{\text{lequ}}(0)^{1-\text{inst.}} &= -i\lim_{k\to 0}\int d^4x e^{ikx}\left\langle 0\left| T\left\{\frac{1}{32\pi^2}G\widetilde{G}(x), \frac{C^{(1)}_{\text{lequ}}}{\Lambda^2_{\not{CP}}}\mathcal{O}^{(1)}_{\text{lequ}}(0)\right\}\right| 0\right\rangle ,\\ &= e^{-i\theta_{\text{QCD}}}\int d^4x_0 \int\frac{d\rho}{\rho^5}d_N(\rho)\int \mathcal{D}H\mathcal{D}H^\dagger\mathcal{D}L\mathcal{D}\bar{L}\mathcal{D}e\mathcal{D}\bar{e}\, e^{-S_0[H,H^\dagger]}\, e^{-S_0[L,\bar{L}]}\, e^{-S_0[e,\bar{e}]}\end{aligned}$$

$$\times \int \prod_{f=1}^{3} \left(\rho^2\, d\xi^{(0)}_{u_f} d\xi^{(0)}_{d_f} d^2\bar{\xi}^{(0)}_{Q_f}\right) e^{\int d^4x(\bar{Q}Y_{\mathrm{u}}\widetilde{H}u+\bar{Q}Y_{\mathrm{e}}Hd+\bar{L}Y_{\mathrm{e}}He+\mathrm{h.c.})(x)} \tag{8.41}$$
$$\times \frac{1}{32\pi^2}\int d^4x\, G\widetilde{G}(x)\left(\frac{C^{(1)}_{\mathrm{lequ}}}{\Lambda^2_{\not{CP}}}\bar{L}e\bar{Q}u(0)+\mathrm{h.c.}\right).$$

As previously, we will now expand the exponential of the action containing the fermion and Higgs field. We expand the exponential over the quark Yukawa couplings in the zero modes as before and neglect the quark non-zero modes. Then, as is usually done in perturbation theory, we expand the exponential of the lepton Yukawa interaction order by order in the small Yukawa coupling. Expanding the exponential to first order will be sufficient to obtain a non-vanishing result

$$\chi^{(1)}_{\mathrm{lequ}}(0)^{1\text{-inst.}} = e^{-i\theta_{\mathrm{QCD}}}\int d^4x_0\int\frac{d\rho}{\rho^5}d_N(\rho)\int \mathcal{D}H\mathcal{D}H^\dagger\mathcal{D}L\mathcal{D}\bar{L}\mathcal{D}e\mathcal{D}\bar{e}\, e^{-S_0[H,H^\dagger]}$$
$$\times\, e^{-S_0[L,\bar{L}]}\, e^{-S_0[e,\bar{e}]}\prod_{f=1}^{3}\left(\rho^2\, d\xi^{(0)}_{u_f}d\xi^{(0)}_{d_f}d^2\bar{\xi}^{(0)}_{Q_f}\right)\int d^4x_1d^4x_2d^4x_3d^4x_4d^4x_5$$
$$\times\frac{1}{6!}\Bigg[\sum_{\substack{\text{perm. over}\\ \text{fermion fields}}}\bar{\xi}^{(0)}_{Q^I_{i_1}}(\bar{\psi}^{(0)}Y_{\mathrm{u},i_1j_1}\widetilde{H}^IP_R\psi^{(0)})(x_1)\xi^{(0)}_{u_{j_1}}\quad \bar{\xi}^{(0)}_{Q^J_{i_2}}(\bar{\psi}^{(0)}Y_{\mathrm{u},i_2j_2}\widetilde{H}^JP_R\psi^{(0)})(x_2)\xi^{(0)}_{u_{j_2}}$$
$$\times\,\bar{\xi}^{(0)}_{Q^K_{k_1}}(\bar{\psi}^{(0)}Y_{\mathrm{d},k_1l_1}H^KP_R\psi^{(0)})(x_3)\xi^{(0)}_{d_{l_1}}\quad\bar{\xi}^{(0)}_{Q^L_{k_2}}(\bar{\psi}^{(0)}Y_{\mathrm{d},k_2l_2}H^LP_R\psi^{(0)})(x_4)\xi^{(0)}_{d_{l_2}} \tag{8.42}$$
$$\times\,\bar{\xi}^{(0)}_{Q^M_{k_3}}(\bar{\psi}^{(0)}Y_{\mathrm{d},k_3l_3}H^MP_R\psi^{(0)})(x_5)\xi^{(0)}_{d_{l_3}}\int d^4x\frac{G\widetilde{G}(x)}{32\pi^2}\left(\frac{C^{(1)}_{\mathrm{lequ},mnop}}{\Lambda^2_{\not{CP}}}\left(\bar{L}^N_me_n\right)\epsilon_{NO}\right.$$
$$\times\left.\bar{\xi}^{(0)}_{Q^O_o}(\bar{\psi}^{(0)}P_R\psi^{(0)})\xi^{(0)}_{u_p}\right)(0)\Bigg]\int d^4x_6\left(\bar{e}_qY^\dagger_{\mathrm{e},qr}H^{\dagger,P}L^P_r\right)(x_6)\,.$$

Note that in comparison to the computation of $\mathcal{O}^{(1)}_{\mathrm{quqd}}$, an extra down Yukawa coupling is needed to get a non-vanishing Grassmann integral, because the down-quark bilinear in $\mathcal{O}^{(1)}_{\mathrm{quqd}}$ is replaced with the lepton bilinear in $\mathcal{O}^{(1)}_{\mathrm{lequ}}$. In the next step, we will perform the integration in the path integral over the Higgs and lepton fields, as well as the zero mode integrals. Using the definition of the lepton propagator

$$\int\mathcal{D}\psi\mathcal{D}\bar{\psi}\,e^{-S_0[\psi,\bar{\psi}]}\,\psi_I(x_1)\bar{\psi}_J(x_2)\equiv\Delta_F(x_1-x_2)\,\delta_{IJ}\,, \tag{8.43}$$

the lepton fields are contracted to form a loop.[7] The resulting expression reads

$$\chi^{(1)}_{\mathrm{lequ}}(0)^{1\text{-inst.}} = \frac{1}{2\Lambda^2_{\not{CP}}}\underbrace{e^{-i\theta_{\mathrm{QCD}}}\epsilon^{i_1i_2m}\epsilon^{j_1j_2n}Y_{\mathrm{u},i_1j_1}Y_{\mathrm{u},i_2j_2}C^{(1)}_{\mathrm{lequ},opmn}Y^\dagger_{\mathrm{e},po}\det Y_{\mathrm{d}}}_{\equiv I^{(1)}_{\mathrm{lequ}}}$$

[7] The indices I, J represent all internal indices, like the flavour and $SU(2)$ gauge group indices.

$$\times 3! \int d^4x_0 \int \frac{d\rho}{\rho^5} d_N(\rho)\rho^6 \mathcal{I}^2 \int d^4x_5 d^4x_6 \left(\bar{\psi}^{(0)} P_R \psi^{(0)}\right)(x_5)\Delta_H(x_5 - x_6) \tag{8.44}$$
$$\times \operatorname{tr}\left(P_R \Delta_F(x_6 - 0) P_L \Delta_F(0 - x_6)\right)\left(\bar{\psi}^{(0)} P_R \psi^{(0)}\right)(0)\, \epsilon_{OP}\epsilon^{PO} \int d^4x \frac{G\widetilde{G}(x)}{32\pi^2}\,.$$

The final result is obtained by adding the anti-instanton contribution, which leads to the complex conjugate invariants appearing with the opposite sign in the final result. Thus, the final result is again proportional to the CP-odd invariant of the semileptonic operator

$$\operatorname{Im}\left(I^{(1)}_{\text{lequ}}\right) = \operatorname{Im}\left[e^{-i\theta_{\text{QCD}}}\epsilon^{i_1 i_2 m}\epsilon^{j_1 j_2 n} Y_{\text{u},i_1 j_1} Y_{\text{u},i_2 j_2} C^{(1)}_{\text{lequ},opmn} Y^\dagger_{\text{e},po} \det Y_{\text{d}}\right] = \mathcal{I}^0_{0000}\left(C^{(1)}_{\text{lequ}}\right), \tag{8.45}$$

that we have defined in Sec. 8.2.1 multiplied by a complicated integral. In App. 8.A.2, we evaluate the integrals in Eq. (8.44), where we find a divergent loop integral due to the lepton loop. We explicitly verify that working in renormalised perturbation theory of the SMEFT, the appropriate counterterm cancels this divergence.

In addition, we can also apply the NDA estimate of Ref. [242] to this result and find a suppression of $(4\pi)^{-8}$ matching the π suppression of the final result obtained in Eq. (8.81) with a numerical factor $\simeq 1/(450\pi^8)$. Taking into account the combinatoric factors as well as the additional factors from the unbroken $SU(2)$ group, the NDA estimate of 4^{-8} is approximately half of the full result.

This analysis can be repeated for all other operators in the SMEFT following the same procedure. We present calculations for the insertion of the gluon dipole operator $\mathcal{O}_{\text{dG}}$ in App. 8.A.3, that will also be considered in a phenomenological study in Sec. 8.4. For some SMEFT operators, the leading contribution might not arise by directly connecting all their fermion legs to the instanton background through their zero modes. Indeed, considering non-zero modes of the quarks in the effective operators is also needed to obtain the invariants with more powers of Yukawa couplings introduced in Sec. 8.2.1. We will discuss the calculations in these cases next.

8.3.5 Higher-Order Invariants and Selection Rules

Throughout the last sections we have explicitly shown that the invariants constructed in Sec. 8.2.1 naturally appear in instanton computations. However, we found that the contributions we computed only come with the invariant least suppressed in the Yukawa couplings. We expect the higher-order invariants to appear by computing higher-loop diagrams, where more Yukawa couplings insertions are generated through fermion-Higgs couplings. We have depicted such a diagram for the 4-quark operator $\mathcal{O}^{(1)}_{\text{quqd}}$ in Fig. 8.1b. One has to take care while performing those computations, because Yukawa interactions mixing the zero and non-zero modes of the fermions charged under the instanton group have to be kept in the path integral. In the invariants, these interactions will connect the determinant-like structure generated by the zero modes by a matrix product to the further Yukawa insertions due to fermion propagators.

Explicitly performing this calculation is beyond the scope of this work but we will comment on how these calculations work in principle. Instead of just including the quark zero modes in the calculations, one would have to include the non-zero mode interactions in the action as well. These should be treated perturbatively as was done for the leptons in Sec. 8.3.4. As a consequence, the non-zero mode part of the path integral no longer comes in a Gaussian form that allows us to simply integrate of them as done in Eq. (8.25). Hence, 't Hooft's computations have to be redone without performing the non-zero mode integration, which amounts to removing the factor of $e^{0.292 N_f}$ from the instanton density in Eq. (2.152) and treating the non-zero modes of the coloured fields as perturbations around the instanton background. This leads to further questions about the propagation of these modes in an instanton background. If the propagator is not simply that of the free quark fields, the computations could be further complicated.

In summary, the invariants with more powers of Yukawa couplings are generated in computations where the Yukawa interactions contain mixed terms with zero- and non-zero modes of the quarks and the terms with only non-zero modes. Then, matrix products of the extra Yukawa couplings are generated by Kronecker deltas upon contracting the quark non-zero modes to flavourful propagators in the perturbative calculation (c.f. the calculation with the semi-leptonic operator in Sec. 8.3.4). The zero mode indices remain contracted in a determinant-like manner via Levi-Civita symbols.

In addition, using flavour invariants we can understand why operators invariant under the Abelian part $U(1)^5$ of the flavour group (shown in Table 8.1) cannot enter through zero mode contributions in instanton calculations. One such operator is $\mathcal{O}_{\mathrm{Hq}}^{(1)}$, which is invariant under flavour-universal $U(1)_Q$ rephasings $Q \to e^{i\alpha_Q} Q$ (and trivially under the remaining $U(1)^4$ rephasings). Because the operator is rephasing invariant, other flavourful objects besides the Wilson coefficient are needed to counteract the rephasing of $e^{-i\theta_{\mathrm{QCD}}}$ that necessarily appears in instanton calculations. Due to the linearity of the flavour invariants in the Wilson coefficient, this object can only be constructed by SM Yukawa couplings. There are two options to construct a flavour invariant given these constraints. The object counteracting the rephasing of $e^{-i\theta_{\mathrm{QCD}}}$ can either be $\det Y_{\mathrm{u}} Y_{\mathrm{d}}$ with the Wilson coefficient appearing in a trace invariant or a determinant-like invariant of the Wilson coefficient where, even at lowest order, the Wilson coefficient multiplies one of the Yukawa couplings (c.f. Eq. (8.11)).[8] As we have discussed previously, both traces and matrix products can only appear through propagators in perturbative calculations of the non-zero modes of quarks around the instanton background. Hence, the flavour invariants imply a selection rule on all operators that are invariant under flavour-universal $U(1)^3_{Q,u,d}$ rephasings to only contribute in instanton calculations when the non-zero modes of the fermions are considered.

In general, the flavour invariants can be used to systematise the instanton computations by understanding how the contribution from any SMEFT operator will look like before performing any computations, as we have anticipated in Sec. 8.3.2. The invariants also give an idea about which contribution is the most important by counting insertions of Yukawa couplings and loop factors, which usually come with the higher-order invariants. Therefore, using the invariants for instanton computations in the presence of effective operators enables the refinement of the NDA estimates of instanton effects in the spirit of Ref. [242].

[8] These two types of invariants are equivalent as we show explicitly in Eq. (8.13) for the operator $\mathcal{O}_{\mathrm{Hq}}^{(1)}$ and all arguments presented here work for both forms.

8.4 Constraints on Dimension-6 CP-violating Operators

We can utilise the results obtained in the previous sections to set bounds on the scale $\Lambda_{\not{CP}}$ associated with dimension-six CP violating operators. To perform the integrals over the instanton size ρ, we have to assume a specific realisation for the modification of QCD at a scale $\Lambda_{\rm SI}$, such that instanton effects are enhanced, while the 1-instanton approximation still remains valid. As we will see below, the induced shift in $\bar{\theta}$ will parametrically go as $\Lambda_{\rm SI}^2/\Lambda_{\not{CP}}^2$, which can be much bigger than similar effects in ordinary QCD scaling like $\Lambda_{\rm QCD}^2/\Lambda_{\not{CP}}^2$. We will set bounds on the ratio $\Lambda_{\rm SI}/\Lambda_{\not{CP}}$ by assuming that the induced theta term in the small instanton background saturates the experimental bound obtained from the neutron EDM, $\bar{\theta} \lesssim 10^{-10}$ [43]. Using the determinant-like flavour invariants derived in the last section will allow us to easily assess different flavour scenarios and take into account off-diagonal contributions of Wilson coefficients appearing due to the CKM matrix.

To achieve an enhancement of the strong gauge coupling, we will consider two different UV models modifying the UV dynamics of QCD. We will briefly review them here.

Product Group Models In the first model, we consider an extension of the gauge group of QCD to a product of several $SU(3)$ groups, which is subsequently spontaneously broken by the VEVs of some scalar fields σ. In such a model, the instanton density $d_N(\rho)$ is modified by an exponential factor

$$d_N(\rho) \to d_N(\rho)\, e^{-2\pi^2\rho^2 \sum_\sigma |\langle\sigma\rangle|^2}\,, \tag{8.46}$$

where the sum extends over all the scalars σ that Higgs the gauge group. The VEV of the scalars provides a natural cutoff $\sim 1/|\langle\sigma\rangle|$ for the integration over the instanton size ρ. For definiteness, we consider the product group model introduced in Refs. [240, 344], where the gauge group $SU(3)_1 \times SU(3)_2 \times \cdots \times SU(3)_k$ is Higgsed to the diagonal $SU(3)_c$ via bifundamental scalars σ. When the theory is eventually matched to QCD at a scale M, where all the heavy gluons from the theory can be integrated out, the matching condition reads as follows

$$\frac{1}{g_s^2(M)} = \sum_{i=1}^{k} \frac{1}{g_i^2(M)}\,. \tag{8.47}$$

Hence, to remain compatible with the QCD coupling at low energies each of the gauge couplings g_i has to be larger than the strong coupling g_s at the matching scale M. In particular, the higher the total number k of $SU(3)$ subgroups appearing in the product group, the stronger the coupling in each of the $SU(3)$ subgroups has to be.

5D Instantons In the second model we consider the strong coupling is enhanced by uplifting the BPST instanton presented in Eq. (2.129) to a compact extra dimension of size R [360], which modifies the running of the effective gauge coupling in Eq. (2.151) above the compactification scale $1/R$. The effective action then becomes

$$S_{\rm eff} \simeq \frac{8\pi^2}{g^2(1/R)} - \frac{R}{\rho} + b_0 \ln\frac{R}{\rho}\,, \tag{8.48}$$

where b_0 is the 1-loop coefficient of the QCD β-function and the linear term R/ρ is due to additional contributions in Eq. (2.146) from the Kaluza–Klein modes. This leads to a modification of the instanton density by an amount

$$d_N(\rho) \to d_N(\rho)\, e^{R/\rho}\,. \tag{8.49}$$

The dilute instanton gas approximation holds true in computations of the topological susceptibility in this model as longs as the 5D perturbativity condition

$$\Lambda_{\mathrm{SI}} R \lesssim \frac{24\pi^2}{g^2}\,, \tag{8.50}$$

is enforced, where Λ_{SI} is identified with the cut-off scale of the 5D gauge theory.

8.4.1 Bounds from Induced $\bar{\theta}$

As discussed in Sec. 8.3, new sources of CP violation in the SMEFT can induce a shift in $\bar{\theta}$, which leads to observable effects such as a non-vanishing neutron EDM. In principle, all CP-violating operators in the SMEFT can contribute to an induced theta term, where the form of the contributions are dictated by the invariants presented in Ref. [3]. Hence, due to the different flavour structures necessary to built invariants for the different operators, there are only a few invariants that contribute at the leading order.

In the following, we consider three different flavour scenarios to study their impact on the constraints obtained from the neutron EDM bound on the induced θ-angle. We will briefly introduce them here.

1. The simplest flavour scenario we consider is the **anarchic flavour scenario**, in which all entries of the Wilson coefficients have an $\mathcal{O}(1)$ value. Compared to the SM, this will in particular lead to large flavour-changing interactions.

2. A slightly more restrictive flavour assumption is the **MFV scenario**. As we have noted earlier, in the SM the only breaking of the $U(3)^5$ flavour symmetry of the fermion kinetic term is due to the SM Yukawa couplings. Taking the Yukawa couplings to be spurions under this symmetry (c.f. Table 8.1), makes the Lagrangian formally invariant under this approximate symmetry. In MFV we assume that also in the UV sector, that generates the non-renormalisable operators of the SMEFT, the only couplings breaking the $U(3)^5$ flavour symmetry are the SM Yukawa couplings. Thus, all SMEFT Wilson coefficients are polynomials in the Yukawa couplings dictated by the spurious transformations of the Wilson coefficients under the flavour group.

3. Lastly, we consider an **FN scenario** that offers an explanation for the size of the SM lepton and quark masses as well as the parameters in the CKM matrix. We have already introduced this model in Chap. 4 to obtain a single parameter description of the SM and SMEFT flavour sector, which allowed us to organise the SMEFT flavour invariants, and in Chap. 6 in combination with a PQ mechanism to generate flavourful ALP couplings.

We will briefly introduce the main aspects of the mechanism in more details here to set the stage for the analysis of the flavour invariants. In the FN scenario, the SM field content is extended by a complex scalar field ϕ which is a singlet under the SM gauge group and has charge -1 under a new global $U(1)$ symmetry. Constructing a Lagrangian invariant under the SM gauge group and the newly postulated $U(1)$ yields

$$\mathcal{L} = -\left(\frac{\phi^\star}{\Lambda_{\rm FN}}\right)^{q_{Q_i}+q_{u_j}} C^u_{ij}\bar{Q}_i\tilde{H}u_j - \left(\frac{\phi^\star}{\Lambda_{\rm FN}}\right)^{q_{Q_i}+q_{d_j}} C^d_{ij}\bar{Q}_i H d_j - \left(\frac{\phi^\star}{\Lambda_{\rm FN}}\right)^{q_{L_i}+q_{e_j}} C^e_{ij}\bar{L}_i H e_j\,, \tag{8.51}$$

where the FN charges of the left-handed fermions Q, $u^\dagger$, $d^\dagger$, L, $e^\dagger$ are denoted as q_Q, q_u, q_d, q_L, q_e, respectively, $q_H = 0$, $\Lambda_{\rm FN}$ is the effective scale where the Froggatt–Nielsen scenario is UV completed and the coefficients $C^{u,d,e}_{ij}$ are $\mathcal{O}(1)$ complex numbers. Eventually, the global $U(1)$ symmetry is broken by the VEV of the complex scalar, which yields hierarchical Yukawa couplings as powers of $\lambda = \frac{\langle\phi\rangle}{\Lambda_{\rm FN}} \sim 0.2$ dictated by the FN charges. One set of charge assignments that can reproduce the SM Yukawa couplings to large accuracy is

$$q_Q = \{3,2,0\}, \quad q_u = \{5,2,0\}, \quad q_d = \{4,3,3\}\ , \tag{8.52}$$

for the quarks and

$$q_L = \{9,5,3\}, \quad q_e = \{0,0,0\}\ , \tag{8.53}$$

for the leptons. This construction can be extended to the effective operators of the SMEFT [361], resulting in hierarchical entries for the Wilson coefficients.

We begin by identifying the leading order invariants amongst those given in Sec. 8.2. This can be easily achieved by studying the FN scaling of the invariant with the least number of Yukawa matrices for each operator. Consider the topological susceptibility of QCD, $\chi(0) \propto K_\theta$, e.g., which scales as $\propto \lambda^{27}$. This compares with the SMEFT invariants in Sec. 8.2.1 which scale as

$$\mathcal{I}_{0000}(C_{\rm uH}),\, \mathcal{A}^{0000}_{0000}(C^{(1,8)}_{\rm ququd}),\, \mathcal{B}^{0000}_{0000}(C^{(1,8)}_{\rm ququd}) \propto \lambda^{27}\ , \tag{8.54}$$

$$\mathcal{I}_{1100}(C^{(1,3)}_{\rm Hq}),\, \mathcal{I}^{0}_{0000}(C^{(1,3)}_{\rm lequ}) \propto \lambda^{33}\ . \tag{8.55}$$

This scaling helps to determine which invariants are the least suppressed and hence phenomenologically the most interesting. For instance, Eqs. (8.54) and (8.55) indicate that the operators $\mathcal{O}_{\rm uH}$ and $\mathcal{O}^{(1,8)}_{\rm ququd}$ lead to larger effects compared to $\mathcal{O}^{(1,3)}_{\rm Hq}$ or $\mathcal{O}^{(1,3)}_{\rm lequ}$, i.e. if the Wilson coefficients are assumed to be of the same order (reduced by the appropriate λ scaling in the FN scenario), the contribution of the operator $\mathcal{O}^{(1,8)}_{\rm ququd}$ (or $\mathcal{O}_{\rm uH}$) to $\theta_{\rm ind}$ dominates over that of $\mathcal{O}^{(1,3)}_{\rm lequ}$ (or $\mathcal{O}^{(1,3)}_{\rm Hq}$). This can also be understood from the diagrams in Fig. 8.1a and Fig. 8.1d – the latter diagram, corresponding to the semi-leptonic operator, contains additional loops and Yukawa couplings compared to the former diagram, corresponding to the 4-quark operator, and the leading order contribution from $\chi(0)$.

Below, we study in more detail how these invariants contribute to the shift of the axion potential minimum, $\theta_{\rm ind}$, for the two leading-order operators – the 4-quark operator $\mathcal{O}^{(1)}_{\rm quqd}$ and the dipole operator $\mathcal{O}_{\rm dG}$, as well as the sub-leading semi-leptonic operator $\mathcal{O}^{(1)}_{\rm lequ}$.

For this analysis, the MFV (at leading order) and FN flavour scenarios result in the same scaling for the Wilson coefficients, which occurs because we only consider the contribution from chirality-flipping operators to one observable. For instance, the scaling of $\mathcal{O}^{(1)}_{\rm quqd}$ is

$$C^{(1)}_{{\rm quqd},ijkl} \overset{\rm MFV}{\sim} c_1 Y_{{\rm u},ij} Y_{{\rm d},kl} + \mathcal{O}(Y^3_{\rm u,d})\,, \qquad C^{(1)}_{{\rm quqd},ijkl} \overset{\rm FN}{\sim} c_{1,ijkl} \lambda^{q_{Q_i}+q_{u_j}+q_{Q_k}+q_{d_l}}\,, \tag{8.56}$$

where c_1 are $\mathcal{O}(1)$ coefficients. Since by the FN construction, Eq. (8.51), $Y_{\rm u} \sim \lambda^{q_Q+q_u}$ and $Y_{\rm d} \sim \lambda^{q_Q+q_d}$, we explicitly see the same scaling in both scenarios. Therefore, in the following we will only present constraints on $\Lambda_{\not{CP}}$ (for a given $\Lambda_{\rm SI}$) under the anarchic and the MFV scenario for the considered operators.

Four-Quark Operators For the 4-quark operator $\mathcal{O}^{(1)}_{\rm quqd}$, the topological susceptibility is computed in App. 8.A.1, where the final result up to the integration over the instanton size can be found in Eq. (8.68). Performing the integral over ρ in the product group model $SU(3)^k \to SU(3)_c$ and setting $|\langle\sigma\rangle| = \Lambda_{\rm SI}$, we obtain

$$\theta_{\rm ind} = \frac{16\pi^2}{5(b_0-6)K_\theta}\left(\mathcal{A}^{0000}_{0000}\left(C^{(1)}_{\rm quqd}\right) + \mathcal{B}^{0000}_{0000}\left(C^{(1)}_{\rm quqd}\right)\right)\frac{\Lambda^2_{\rm SI}}{\Lambda^2_{\not{CP}}}\,, \tag{8.57}$$

where $b_0 = 13/2$ for the first subgroup $SU(3)_1$, $b_0 = 10$ for the middle $k-2$ subgroups $SU(3)_2, \ldots SU(3)_{k-1}$ and $b_0 = 21/2$ for the last subgroup $SU(3)_k$ of the product gauge group, yielding an additional factor of 2 on the right-hand side of Eq (8.57). In the case of 5D instantons, we obtain

$$\theta_{\rm ind} = \frac{2}{5K_\theta}\left(\mathcal{A}^{0000}_{0000}\left(C^{(1)}_{\rm quqd}\right) + \mathcal{B}^{0000}_{0000}\left(C^{(1)}_{\rm quqd}\right)\right)\frac{\Lambda^2_{\rm SI}}{\Lambda^2_{\not{CP}}}\,. \tag{8.58}$$

As a consequence of Higgsing the product gauge group, the model has a natural IR cutoff on the instanton size ρ, which leads to a mild dependence on the β function coefficient, b_0 in Eq. (8.57). In contrast, the dependence of the instanton density of the 5D instanton model in Eq. (8.49) on the instanton size implies that the integral over ρ is dominated by instantons of size $\rho \sim 1/\Lambda_{\rm SI}$. Therefore, all the susceptibilities for the 5D model only depend on $\Lambda_{\rm SI}$, up to an overall factor. This factor cancels when taking the ratio of susceptibilities, implying that $\theta_{\rm ind}$ is independent of the β function coefficient, b_0. The constraints arising from Eqs. (8.57) and (8.58) on the scale of CP violation $\Lambda_{\not{CP}}$ as a function of the scale of small instantons $\Lambda_{\rm SI}$ are shown in Fig. 8.2, where for the product group model, we use $b_0 = 13/2$ since it gives the most stringent constraints. For easy comparison, we will use the same value of b_0 to constrain both the semi-leptonic and gluon dipole operators. In the anarchic flavour scenario, we find that $\Lambda_{\not{CP}} \gtrsim 10^{10}(10^{11})\,\Lambda_{\rm SI}$ for the 5D (product group) model. As expected, the constraint is relaxed

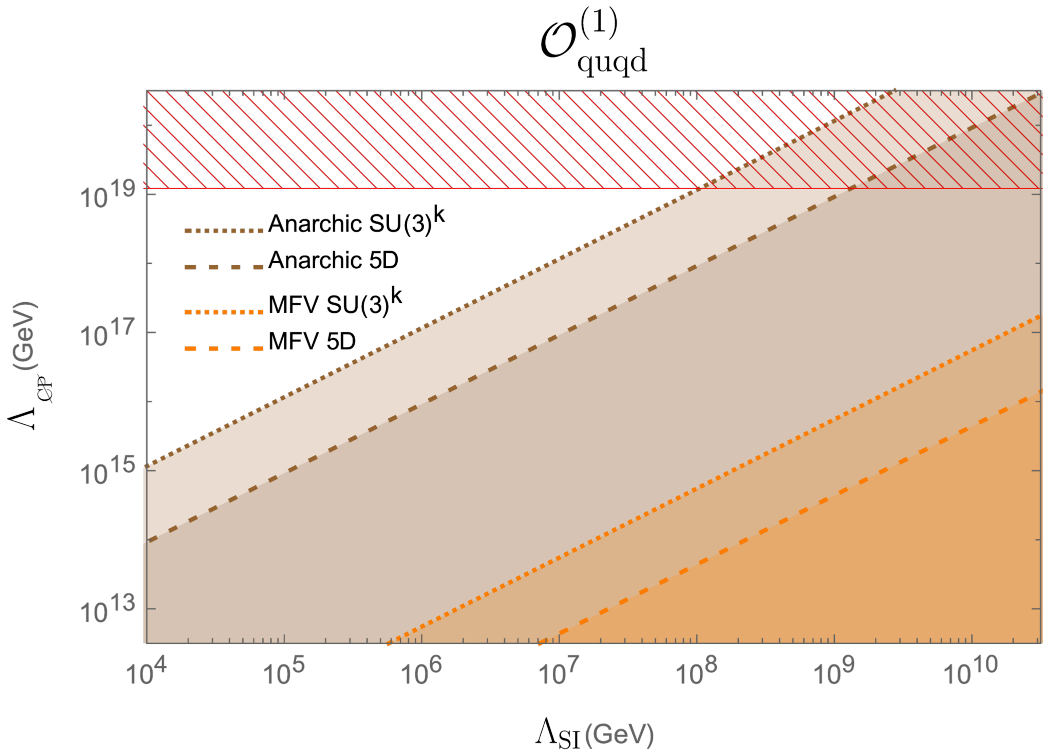


Figure 8.2: Limits on the UV scale $\Lambda_{\not{CP}}$ of the 4-quark operator $\mathcal{O}^{(1)}_{\rm ququd}$ in different flavour scenarios as a function of the small instanton scale $\Lambda_{\rm SI}$. The shaded regions are excluded by the non-observation of the neutron EDM. The striped red region, which corresponds to scales above the Planck mass, is plotted for reference.

in the MFV scenario due to the additional Yukawa suppression of the Wilson coefficients – $\Lambda_{\not{CP}} \gtrsim 5 \times 10^5 (10^6)\, \Lambda_{\rm SI}$ for the 5D (product group) model, which differs exactly by a factor of $\sim \sqrt{y_{\rm u} y_{\rm d}}$, as indicated by Eq (8.5). This matches the MFV scenario considered in Ref. [337], up to an overall factor due to the Higgs doublet structure. In addition, the invariants help us to easily incorporate off-diagonal Yukawa couplings which improves the previous estimate of $\theta_{\rm ind}$ in Ref. [337] by $\sim 6\%$.

Semi-Leptonic Operator For the 4-fermion operator $\mathcal{O}^{(1)}_{\rm lequ}$, the susceptibility up to the integration over the instanton size can be found in Eq. (8.81). In the case of the product group model, performing the integral over ρ gives

$$\theta_{\rm ind} = \frac{\mathcal{I}^0_{0000}(C^{(1)}_{\rm lequ})}{(b_0-6)K_\theta}\left[\frac{11}{25} + \frac{6}{5}\left(\log\left(\frac{\Lambda_{\not{CP}}}{\Lambda_{\rm SI}}\right) + \gamma_{\rm E} - \log 4\pi\right) + \frac{3}{5}\Psi\left(\frac{b_0}{2} - 3\right)\right]\frac{\Lambda^2_{\rm SI}}{\Lambda^2_{\not{CP}}}\,, \tag{8.59}$$

where $\Psi(z)$ is the digamma function and γ_E is Euler's constant, while in the 5D instanton model we obtain

$$\theta_{\rm ind} = \frac{\mathcal{I}^0_{0000}(C^{(1)}_{\rm lequ})}{8\pi^2 K_\theta}\left[\frac{11}{25} + \frac{6}{5}\left(\log\left(\frac{\Lambda_{\not{CP}}}{\Lambda_{\rm SI}}\right) + \gamma_{\rm E} - \log 2\right)\right]\frac{\Lambda^2_{\rm SI}}{\Lambda^2_{\not{CP}}}\,. \tag{8.60}$$

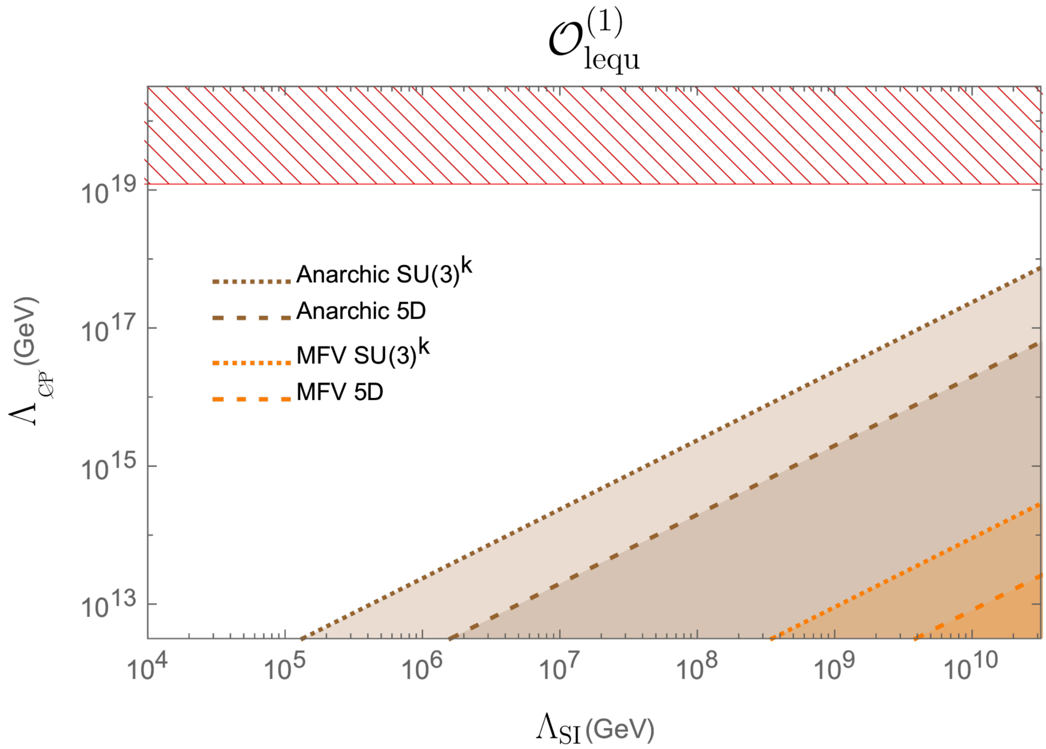


Figure 8.3: Limits on the UV scale $\Lambda_{\not{CP}}$ of the semi-leptonic operator $\mathcal{O}^{(1)}_{\rm lequ}$ in different flavour scenarios as a function of the small instanton scale $\Lambda_{\rm SI}$. The shaded regions are excluded by the non-observation of the neutron EDM. The striped red region, which corresponds to scales above the Planck mass, is plotted for reference.

We present the constraints arising from Eqs. (8.59) and (8.60) in Figure 8.3. As expected, the constraints in this case are much weaker than for the 4-quark operator, because the invariant is more suppressed by the lepton Yukawas, an additional loop factor appears in the computation and more quark Yukawas have to appear in the determinant-like structure of the invariant to close up all of the fermion legs appearing in the flower diagrams. For the anarchic and MFV flavour scenarios, we obtain $\Lambda_{\not{CP}} \gtrsim 10^6 (10^7)\, \Lambda_{\rm SI}$ and $\Lambda_{\not{CP}} \gtrsim 5 \times 10^3 (10^4)\, \Lambda_{\rm SI}$, respectively, for the 5D (product group) model. From Eq. (8.10), we see that the largest term in $\mathcal{I}^0_{0000}(C^{(1)}_{\rm lequ})$ is approximately $\sim K_\theta\, y_\tau / y_{\rm u}$ for the anarchic case ($C^{(1)}_{\rm lequ} \sim \mathcal{O}(1)$), and $\sim K_\theta\, y_\tau^2$ for the MFV scenario ($C^{(1)}_{{\rm lequ},NmLk} \sim Y_{{\rm e},Nm} Y_{{\rm u},Lk}$). This results in a difference by a factor of $\sim \sqrt{y_{\rm u}\, y_\tau}$ between the two flavour scenarios. In comparison to the result for the 4-quark operator, the difference can again be understood in terms of a loop factor and different Yukawa couplings entering the invariants $\mathcal{A}^{0000}_{0000}(C^{(1)}_{\rm quqd})$, $\mathcal{B}^{0000}_{0000}(C^{(1)}_{\rm quqd})$ and $\mathcal{I}^0_{0000}(C^{(1)}_{\rm lequ})$ – for MFV, there is a relative factor of $\sim \sqrt{y_\tau^2/16\pi^2} \equiv \sqrt{\lambda^6/16\pi^2}$ whereas for the anarchic case the factor is $\sim \sqrt{y_\tau y_{\rm d}/16\pi^2}$.

Gluon Dipole Operator Next, we consider the gluon dipole operator $\mathcal{O}_{\rm dG} = (\bar{Q}\sigma^{\mu\nu} T^A d) H\, G^A_{\mu\nu}$. This operator contributes to the topological susceptibility at the same order as $\mathcal{O}^{(1,8)}_{\rm quqd}$, and has the same functional form in terms of instanton parameters. The flavour structure of this

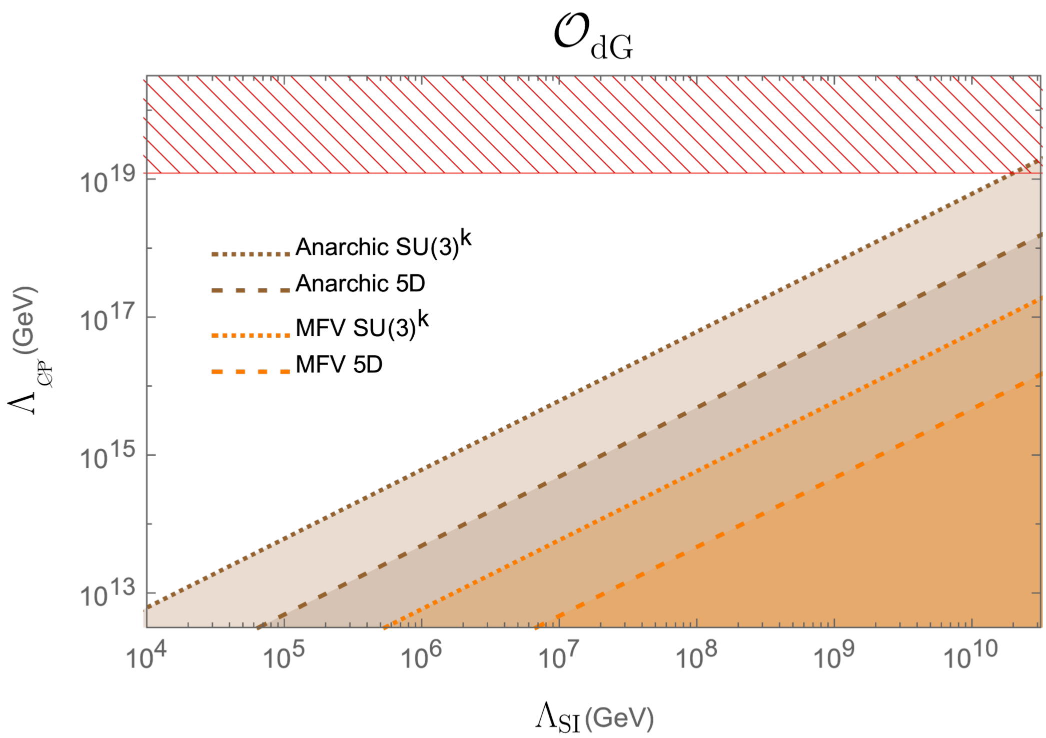


Figure 8.4: Limits on the UV scale $\Lambda_{\not{CP}}$ of the gluon dipole operator $\mathcal{O}_{\rm dG}$ in different flavour scenarios as a function of the small instanton scale $\Lambda_{\rm SI}$. The shaded regions are excluded by the non-observation of the neutron EDM. The striped red region, which corresponds to scales above the Planck mass, is plotted for reference.

operator is similar to $\mathcal{O}_{\rm uH}$ presented in Eq. (8.8), and the leading order invariant is given by

$$\mathcal{I}_{0000}(C_{\rm dG}) \equiv \operatorname{Im}\left[e^{-i\theta_{\rm QCD}}\epsilon^{IJK}\epsilon^{ijk}Y_{{\rm d},Ii}Y_{{\rm d},Jj}C_{{\rm dG},Kk}\det Y_{\rm u}\right], \tag{8.61}$$

The computation of the susceptibility for this operator is given in App. 8.A.3, where the result up to the integration over the zero modes is presented in Eq. (8.87). In this case, the product group model gives the result

$$\theta_{\rm ind} = \frac{\mathcal{I}_{0000}\left(C_{\rm dG}\right)}{K_\theta}\frac{144\pi^2}{5(b_0-6)}\frac{\Lambda_{\rm SI}^2}{\Lambda_{\not{CP}}^2}, \tag{8.62}$$

where b_0 and $|\langle\sigma\rangle|$ are similarly defined as in Eq. (8.57). In the case of the 5D instanton model we obtain

$$\theta_{\rm ind} = \frac{\mathcal{I}_{0000}\left(C_{\rm dG}\right)}{K_\theta}\frac{18}{5}\frac{\Lambda_{\rm SI}^2}{\Lambda_{\not{CP}}^2}. \tag{8.63}$$

The constraints coming from $\theta_{\rm ind}$ in Eqs. (8.62) and (8.63) are presented in Figure 8.4. In the anarchic scenario, the constraint is approximately, $\Lambda_{\not{CP}} \gtrsim 5\times10^7(10^8)\,\Lambda_{\rm SI}$ for the 5D (product group) model. In the anarchic and MFV flavour scenarios we have $C_{{\rm dG},ij}\sim1$ and $C_{\rm dG}\sim Y_{\rm d}$, respectively, resulting in bounds differing by a factor of $\sim\sqrt{y_{\rm d}}$ (see Eq. (8.61)). This is much less pronounced than the difference between $\mathcal{O}^{(1)}_{\rm quqd}$ and $\mathcal{O}^{(1)}_{\rm lequ}$, where a difference of multiple Yukawas arises. It is worth noting that the constraints arising from both the operators $\mathcal{O}^{(1)}_{\rm quqd}$ and $\mathcal{O}_{\rm dG}$ are similar in the MFV scenario, while those from $\mathcal{O}^{(1)}_{\rm lequ}$ are the weakest among the three, as expected.

Finally, note that for simplicity we have assumed that the small instanton-induced θ-angle provides the entire contribution to the neutron EDM. However, in principle, there can be direct contributions to the neutron EDM from the same CP-violating SMEFT operators, which should also be taken into account for a consistent analysis. These contributions from parameters other than $\overline{\theta}$ have been considered in Refs. [5, 44–48] and we expect contributions of a similar size. Due to the random numerical matrix elements in front of the different contributions, we do not expect any large cancellations between the direct and indirect contributions.

Appendices to Chapter 8

8.A Evaluating Loop and Collective Coordinates Integrals

8.A.1 Four-Quark Operator

In the main section of this chapter, we have shown explicitly that the correlation function $\chi^{(1)}_{\text{ququd}}(0)$ with an insertion of the operator $\mathcal{O}^{(1)}_{\text{ququd}}$ is proportional to its determinant-like flavour invariants. There, we have not solved the integral $\mathcal{I}$ and the integral over the instanton centre x_0 appearing in the computation, which we will do explicitly here to obtain analytical results that can be used in the phenomenological analysis performed in Sec. 8.4. The integral $\mathcal{I}$ has previously been calculated in the literature [239, 240, 337] and reads,

$$\begin{aligned}\mathcal{I} &= \epsilon_{IJ}\epsilon^{IJ}\int d^4x_1 d^4x_2\, \big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(x_1)\Delta_H(x_1-x_2)\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(x_2) \qquad (8.64)\\ &= \int d^4x_1 d^4x_2\int d^4k\,\frac{\rho^4}{2\pi^8}\frac{e^{-ikx_1}}{\left(x_1^2+\rho^2\right)^3}\frac{1}{k^2+m_H^2}\frac{e^{ikx_2}}{\left(x_2^2+\rho^2\right)^3} = \frac{\rho^2}{8\pi^4}\int d^4k\,\frac{\left[k\rho\, K_1(k\rho)\right]^2}{(k\rho)^2+(m_H\rho)^2}\,,\end{aligned}$$

where we have plugged the zero mode profile of the fermions in Eq. (2.144) and the (Euclidean) scalar propagator into the first line of Eq. (8.64). The integrals over the Euclidean coordinates $x_1,\ x_2$ are performed using the identity $\int d^4x\, e^{-ikx}/(x^2+\rho^2)^3 = (\pi^2/2)(k/\rho)K_1(k\rho)$, where $K_1(k\rho)$ is the modified Bessel function of the second kind. In the small instanton limit, i.e., $m_H\rho \ll 1$, the integral in Eq. (8.64) evaluates to the following expression

$$\mathcal{I}^{(\text{UV})} \simeq \frac{1}{6\pi^2\rho^2}\,. \qquad (8.65)$$

Secondly, we can evaluate the integrals over the collective coordinate (x_0 in Eq. (8.38)) resulting from the insertion of the 4-quark operator:

$$\int d^4x_0\big(\bar{\psi}^{(0)}P_{R(L)}\psi^{(0)}\,\bar{\psi}^{(0)}P_{R(L)}\psi^{(0)}\big)(0)\Big|_{1-(\text{a})-\text{i.}} = \int d^4x_0\frac{4\rho^4}{\pi^4}\frac{1}{(x_0^2+\rho^2)^6} = \frac{1}{5\pi^2\rho^4}\,. \qquad (8.66)$$

Finally, substituting the results derived in Eqs. (8.64) and (8.66) into Eq. (8.38), we obtain

$$\begin{aligned}\chi^{(1)}_{\text{ququd}}(0) =& \frac{i}{\Lambda^2_{\not{CP}}}\left(\mathcal{A}^{0000}_{0000}\left(C^{(1)}_{\text{ququd}}\right)+\mathcal{B}^{0000}_{0000}\left(C^{(1)}_{\text{ququd}}\right)\right)\times\\ &\times\int\frac{d\rho}{\rho^5}\,d_N(\rho)\rho^6\left[\frac{\rho^2}{8\pi^4}\int d^4k\,\frac{(k\rho)^2K_1^2(k\rho)}{(k\rho)^2+(m_H\rho)^2}\right]^2\frac{2}{5\pi^2\rho^4}\,. \qquad (8.67)\end{aligned}$$

In the small instanton limit, $m_H\rho \ll 1$, the correlator $\chi^{(1)}_{\text{ququd}}(0)$ is given by

$$\chi^{(1)\,(\text{UV})}_{\text{ququd}}(0) = \frac{i}{\Lambda^2_{\not{CP}}}\left(\mathcal{A}^{0000}_{0000}\left(C^{(1)}_{\text{ququd}}\right)+\mathcal{B}^{0000}_{0000}\left(C^{(1)}_{\text{ququd}}\right)\right)\int\frac{d\rho}{\rho^5}\,d_N(\rho)\frac{2!}{(6\pi^2)^2}\frac{2}{5\pi^2\rho^2}\,. \qquad (8.68)$$

The integration over the instanton size, ρ, can be performed once the details of the UV dynamics effects are known that enhance the small instanton effects. Some examples of UV models will be explored in Sec. 8.4.

The results obtained in this appendix also allows for the estimation of higher-order contribution in the EFT with an insertion of the CP-odd phase from $\mathcal{O}^{(1)}_{\text{quqd}}$ and a CP-even parameter from the same operator. This extra insertion of the SMEFT operator can be used to connect two of the petals in a flower diagram in Fig. 8.1 instead of using a Higgs. Hence, in the final result has one power of the integral $\mathcal{I}$, Eq. (8.65), is substituted by one power of the integral in Eq. (8.66). As such, the higher-dimensional contribution will be suppressed by an additional factor of $\left(\frac{\Lambda_{\text{SI}}}{\Lambda_{\not{CP}}}\right)^2$. At the same time, two Yukawa couplings are traded for another Wilson coefficients. As long as one can assume that the flavour suppression by these additional Yukawa couplings is larger than the additional scale suppression $\left(\frac{\Lambda_{\text{SI}}}{\Lambda_{\not{CP}}}\right)^2$, these contributions will be subleading, which is the case even for anarchic flavour scenarios in Sec. 8.4.

8.A.2 Semi-Leptonic Operator

The remaining integrals with an insertion of the semi-leptonic operator $\mathcal{O}^{(1)}_{\text{lequ}}$, that where not solved in the main section, can be evaluated starting from Eq. (8.44) after adding the anti-instanton contribution. The topological susceptibility, $\chi^{(1)}_{\text{lequ}}(0)$ reads

$$\chi^{(1)}_{\text{lequ}}(0) = \frac{i}{\Lambda^2_{\not{CP}}}\mathcal{I}^0_{0000}\left(C^{(1)}_{\text{lequ}}\right)\int\frac{d\rho}{\rho^5}d_N(\rho)\left(3!\,\rho^6\mathcal{I}^2\right)\mathcal{I}_{\text{lequ}}\,, \tag{8.69}$$

where the insertion of $\mathcal{O}^{(1)}_{\text{lequ}}$ appears in the integral $\mathcal{I}_{\text{lequ}}$, defined as

$$\begin{aligned}\mathcal{I}_{\text{lequ}} = \epsilon_{OP}\epsilon^{OP}\int d^4x_0 d^4x_5 d^4x_6\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(x_5)\Delta_H(x_5-x_6)\times\\ \times\,\text{tr}\left(P_R\,\Delta_F(x_6-0)P_L\,\Delta_F(0-x_6)\right)\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(0)\,,\end{aligned} \tag{8.70}$$

which contains a divergent loop integral that needs to be regulated.

Evaluating the Divergent Part of $\mathcal{I}_{\text{lequ}}$ Next, we substitute the (Euclidean) scalar and fermion propagators into Eq. (8.70) to give

$$\begin{aligned}\mathcal{I}_{\text{lequ}} = 2\int d^4x_0\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(0)\\ \times\int d^4x_5\int\frac{d^4k}{(2\pi)^4}\int\frac{d^dq}{(2\pi)^d}\,\text{tr}\left[P_R\frac{\not{q}}{q^2}P_L\frac{\not{q}+\not{k}}{(q+k)^2}\right]\frac{e^{-ikx_5}}{k^2+m_H^2}\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(x_5)\,.\end{aligned} \tag{8.71}$$

Here, we have used the integral representation of the 4-dimensional Dirac delta distribution to eliminate the integration over x_6. We regulate the divergent loop integral by employing dimensional regularisation in the $\overline{\text{MS}}$ scheme in the semi-naive approach [362] of dealing with γ^5 matrices in $d = 4-2\epsilon$ dimensions. We find for the UV-divergent part of the loop integral in $\mathcal{I}_{\text{lequ}}$,

$$\mathcal{I}_{\text{lequ}}^{\text{div.}} = \frac{1}{16\pi^2\epsilon}\left[2\int d^4x_0 d^4x_5 \big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(0)\int \frac{d^4k}{(2\pi)^4}\frac{k^2\,e^{-ikx_5}}{k^2+m_H^2}\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(x_5)\right]. \quad (8.72)$$

This integral contains a UV divergence manifested as a $\frac{1}{\epsilon}$-pole, which can be cancelled by identifying the appropriate counterterms.

Divergence Cancellation and Relation to the SMEFT RGEs. Using the results for the SMEFT RGEs in Ref. [96] we can extract the appropriate counterterm needed to cancel the divergence in $\chi^{(1)}_{\text{lequ}}(0)$. The SMEFT RGEs reveal that the only counterterm that can cancel the divergence in $\chi^{(1)}_{\text{lequ}}(0)$ is the one responsible for the running of the on-shell operator $\mathcal{O}^{(1)}_{\text{quqd}}$ (all other counterterms either have the wrong flavour structure or require additional insertions of gauge couplings). However, since we are requiring the divergence cancellation at the level of correlation functions, which are not invariant under field redefinitions [65, 67], we need to consider the counterterms in an enlarged Green's basis instead. For this particular case, we can verify that the contribution of $\mathcal{O}^{(1)}_{\text{lequ}}$ to the RGE of $\mathcal{O}^{(1)}_{\text{quqd}}$ is fully determined by a Green's basis operator. Considering the Green's basis of Ref. [363], we find [96]

$$C^{(1),\,\text{c.t.}}_{\text{quqd},mnop} \supset -Y_{\text{d},op}\,G^{\text{c.t.}}_{\text{uHD1},\,mn}\,, \qquad G^{\text{c.t.}}_{\text{uHD1},\,mn} = \frac{1}{16\pi^2\,\epsilon}\,C^{(1)}_{\text{lequ},stmn}\,Y^{\dagger}_{\text{e},ts}\,, \quad (8.73)$$

where $G^{\text{c.t.}}_{\text{uHD1},\,mn}$ is the Wilson coefficient of the redundant Green's basis operator $\mathcal{O}_{\text{uHD1}} = \bar{Q}uD^2\tilde{H}$ that is reduced to $\mathcal{O}^{(1)}_{\text{quqd}}$ via field redefinitions – which can be easily verified at this order in the EFT by replacing $D^2\tilde{H}$ with the Higgs EOM. To cancel the $\frac{1}{\epsilon}$-pole in $\chi^{(1),\,\text{div.}}_{\text{lequ}}(0)$, we need to compute the correlation function with an insertion of the Green's basis operator with the counterterm Wilson coefficient

$$\chi^{\text{c.t.}}_{\text{uHD1}}(0)\Big|_{1\text{-inst.}} = -i\lim_{k\to 0}\int d^4x\, e^{ikx}\left\langle 0\left|T\left\{\frac{1}{32\pi^2}G\widetilde{G}(x), \frac{G^{\text{c.t.}}_{\text{uHD1}}}{\Lambda^2_{\not{CP}}}\mathcal{O}_{\text{uHD1}}(0)\right\}\right|0\right\rangle_{1-\text{inst.}}, \quad (8.74)$$

using similar steps to those used previously in Sec. 8.A.1. Eventually, we obtain

$$\chi^{\text{c.t.}}_{\text{uHD1}}(0) = -\frac{i}{\Lambda^2_{\not{CP}}}\,\text{Im}\big(I_{\text{uHD1}}\big)\int \frac{d\rho}{\rho^5}d_N(\rho)\big(3!\,\rho^6\mathcal{I}^2\big)\,\mathcal{I}_{\text{uHD1}}\,, \quad (8.75)$$

where the invariant I_{uHD1}, supplemented by the counterterm in Eq. (8.73), yields

$$\text{Im}\big(I_{\text{uHD1}}\big) = \text{Im}\left[e^{-i\theta_{\text{QCD}}}\epsilon^{i_1i_2m}\epsilon^{j_1j_2n}Y_{\text{u},i_1j_1}Y_{\text{u},i_2j_2}G^{\text{c.t.}}_{\text{uHD1},\,mn}\det Y_{\text{d}}\right] = \frac{1}{16\pi^2\,\epsilon}\mathcal{I}^{0}_{0000}\left(C^{(1)}_{\text{lequ}}\right). \quad (8.76)$$

The integral $\mathcal{I}_{\text{uHD1}}$ reads

$$\mathcal{I}_{\text{uHD1}} = 2\int d^4x_0\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(0)\int d^4x_5\int \frac{d^4k}{(2\pi)^4}\frac{k^2\,e^{-ikx_5}}{k^2+m_H^2}\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(x_5)\,, \quad (8.77)$$

where we have used the fact that the Green's basis operator contains derivatives (in Euclidean space) acting on the Higgs, hence the path integral over the Higgs fields yields

$$\int \mathcal{D}H\mathcal{D}H^\dagger e^{-S_0[H,H^\dagger]} H_I(x_1)\partial^2 H_J^\dagger(x_2) = \partial_{x_2}^2 \Delta_H(x_1 - x_2)\delta_{IJ} = -\int \frac{d^4k}{(2\pi)^4}\frac{k^2 e^{-ik(x_1-x_2)}}{k^2+m_H^2}\delta_{IJ}\,. \tag{8.78}$$

At this point, we have found that the integral $\mathcal{I}_{\text{uHD1}}$ in Eq. (8.77) obtained from including the counterterm is the same as the integral $\mathcal{I}_{\text{lequ}}^{\text{div.}}$ in Eq. (8.72) up to the overall factor $1/(16\pi^2\epsilon)$. Thus, substituting Eqs. (8.76) and (8.77) into Eq. (8.75), one can easily observe that $\chi_{\text{uHD1}}^{\text{c.t.}}(0)$ precisely cancels the $\frac{1}{\epsilon}$-pole in $\chi_{\text{lequ}}^{(1)}(0)$.

Evaluating the finite part of $\mathcal{I}_{\text{lequ}}$ We can also extract the finite contribution of the integration over the loop momentum q in $\mathcal{I}_{\text{lequ}}$

$$\begin{aligned}\mathcal{I}_{\text{lequ}}^{(\text{fin})} &= 2\int d^4x_0 \big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(0)\\ &\times \int d^4x_5 \int \frac{d^4k}{(2\pi)^4}\frac{k^2\, e^{-ikx_5}}{k^2+m_H^2}\left[\frac{1}{8\pi^2}+\frac{1}{16\pi^2}\log\frac{\mu^2}{k^2}\right]\big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(x_5)\,,\end{aligned} \tag{8.79}$$

where μ is the renormalisation scale. As before, we first integrate over x_5 and the instanton centre x_0. The final integral over the momentum k can be performed in the limit of $m_H \to 0$

$$\begin{aligned}\mathcal{I}_{\text{lequ}}^{(\text{fin,UV})} &\simeq \int \frac{d^4k}{(2\pi)^4}\frac{1}{4\pi^2}\left[1+\frac{1}{2}\log\frac{\mu^2}{k^2}\right]\frac{4\rho^4}{\pi^4}\int d^4x_0 \frac{e^{-ikx_0}}{\big(x_0^2+\rho^2\big)^3}\int d^4x_5 \frac{e^{-ik(x_5-x_0)}}{\big((x_5-x_0)^2+\rho^2\big)^3}\\ &= \int \frac{d^4k}{(2\pi)^4}\frac{1}{4\pi^2}\left[1+\frac{1}{2}\log\frac{\mu^2}{k^2}\right]\left[k\rho\, K_1(k\rho)\right]^2 = \frac{1}{20\pi^4\rho^4}\left(\frac{11}{30}+\log\mu\rho+\gamma_{\text{E}}-\log 2\right).\end{aligned} \tag{8.80}$$

Finally, substituting Eq. (8.65) and Eq. (8.80) into Eq. (8.69), the finite part of the topological susceptibility $\chi_{\text{lequ}}^{(1)}(0)$ induced by the operator $\mathcal{O}_{\text{lequ}}^{(1)}$ becomes

$$\chi_{\text{lequ}}^{(1)(\text{fin,UV})}(0) = \frac{i}{\Lambda_{\cancel{CP}}^2}\mathcal{I}_{0000}^0\left(C_{\text{lequ}}^{(1)}\right)\int \frac{d\rho}{\rho^5}d_N(\rho)\frac{3!}{(6\pi^2)^2}\frac{11+30\left(\log\left(\rho\Lambda_{\cancel{CP}}\right)+\gamma_{\text{E}}-\log 2\right)}{600\pi^4\rho^2}\,. \tag{8.81}$$

The dependence on the renormalisation scale μ in Eq. (8.81) has already been removed by performing the RG evolution induced by $C_{\text{lequ}}^{(1)}$, rendering the final result of θ_{ind} independent of the renormalisation scale as expected. The result in Eq. (8.81) will be used in Sec. 8.4.1 to place bounds on the scale $\Lambda_{\cancel{CP}}$.

8.A.3 Gluon dipole operator

In the computation with an insertion of the gluon dipole operator $\mathcal{O}_{\rm dG} = \bar{Q}\sigma^{\mu\nu}T^A d\, H G^A_{\mu\nu}$ in the correlation we set the field strength tensor in $\mathcal{O}_{\rm dG}$ to its instanton background value, while the rest of the calculation proceeds in a similar fashion to the other effective operators. Since, the gluon dipole operator is also a chirality-flipping single bilinear operator, its flavour invariants have a similar form as those of $\mathcal{O}_{\rm uH}$ presented in Eq. (8.8). Following the previous calculations, combining both the instanton and anti-instanton contributions, the topological susceptibility $\chi_{\rm dG}(0)$ can be written as a flavour invariant multiplied by the integral

$$\chi_{\rm dG}(0) = \frac{i}{\Lambda^2_{\not{CP}}}\mathcal{I}_{0000}(C_{\rm dG})\int \frac{d\rho}{\rho^5} d_N(\rho)\; 3!\,\rho^6 \mathcal{I}^2\; \mathcal{I}_{\rm dG}\,, \tag{8.82}$$

where the $\mathcal{O}_{\rm dG}$ operator is included inside the integral $\mathcal{I}_{\rm dG}$, and defined as

$$\mathcal{I}_{\rm dG} = \epsilon_{IJ}\epsilon^{IJ}\int d^4x_0 \int d^4x_3 \big(\bar{\psi}^{(0)}P_R\psi^{(0)}\big)(x_3)\Delta_H(x_3)\big(\bar{\psi}^{(0)}\sigma^{\mu\nu}T^A P_R\psi^{(0)} G^A_{\mu\nu}|_{1-\rm inst.}\big)(0)\,. \tag{8.83}$$

The computation of $\chi_{\rm dG}(0)$ proceeds in the same way as the integral of $\chi^{(1)}_{\rm ququd}(0)$. Plugging the zero modes of fermions (2.144) and gauge fields (2.133) into this expression, the integral $\mathcal{I}_{\rm dG}$ becomes

$$\begin{aligned}\mathcal{I}_{\rm dG} &= \frac{192\rho^6}{\pi^4}\int \frac{d^4k}{(2\pi)^4}\int d^4x_0\int d^4x_3 \frac{e^{ikx_3}}{(x_3^2+\rho^2)^3}\frac{1}{k^2+m_H^2}\frac{e^{-ikx_0}}{(x_0^2+\rho^2)^5} \\ &= \frac{96\rho^6}{\pi^2}\int \frac{d^4k}{(2\pi)^4}\frac{k\rho\, K_1(k\rho)}{(k\rho)^2+(m_H\rho)^2}\int d^4x_0 \frac{e^{-ikx_0}}{(x_0^2+\rho^2)^5} = \frac{1}{16\pi^4}\int d^4k\, \frac{(k\rho)^4 K_1(k\rho)K_3(k\rho)}{(k\rho)^2+(m_H\rho)^2}\,.\end{aligned} \tag{8.84}$$

Here, we have integrated over x_0 and used the following identity

$$\int d^4x_0 \frac{e^{-ikx_0}}{(x_0^2+\rho^2)^5} = \frac{1}{12}\left(\frac{\partial}{\partial\rho^2}\right)^2\int d^4x_0\frac{e^{-ikx_0}}{(x_0^2+\rho^2)^3} = \frac{\pi^2}{24}\left(\frac{\partial}{\partial\rho^2}\right)^2\left[\frac{k}{\rho}K_1(k\rho)\right] = \frac{\pi^2}{96}\left(\frac{k}{\rho}\right)^3 K_3(k\rho)\,, \tag{8.85}$$

where we have used that $\frac{\partial}{\partial\rho^2}\left[\frac{1}{\rho^n}K_n(k\rho)\right] = -\frac{k}{2\rho^{n+1}}K_{n+1}(k\rho)$. As before, we evaluate the last integral in Eq. (8.84) in the small instanton limit, $m_H\rho \ll 1$,

$$\mathcal{I}^{\rm (UV)}_{\rm dG} \simeq \frac{6}{5\pi^2\rho^4}\,. \tag{8.86}$$

Substituting Eqs. (8.65) and (8.86) into Eq. (8.82), we obtain

$$\chi^{\rm (UV)}_{\rm dG}(0) \simeq \frac{i}{\Lambda^2_{\not{CP}}}\mathcal{I}_{0000}(C_{\rm dG})\int \frac{d\rho}{\rho^5}\, d_N(\rho)\frac{3!}{(6\pi^2)^2}\frac{6}{5\pi^2\rho^2}\,, \tag{8.87}$$

which we will use in Sec. 8.4.1 to set bounds on $\Lambda_{\not{CP}}$.

9 Conclusions to Part II and Closing Words

In the second part of the thesis we have studied different aspects of symmetry breaking in ALP EFTs using flavour invariants and the Hilbert series.

In the first third of Part II, we have reformulated the well-known matrix relations that impose shift symmetry on the couplings of the dimension-5 ALP EFT into a flavour-invariant description. The flavour invariants capture the necessary and sufficient conditions for shift symmetry to hold, hence yielding a set of 13 order parameters for shift symmetry in the dimension-5 ALP EFT. They are explicit and algebraic relations, that only depend on the dimension-5 Wilson coefficients and SM Yukawa couplings in a flavour basis-independent way. The order parameters make it clear, that shift symmetry in the dimension-5 ALP EFT is a collective effect induced by the EW gauge interactions, which connect the up- and down-sector of the theory through the left-handed quark doublet. After computing the RGEs of the invariants, we observe that they are a closed set of differential equations. Hence, the set of flavour invariants is closed under RG flow as expected as the shift symmetry captured by the invariants is preserved by RG flow.

We have illustrated different features of the invariants by explicitly performing the matching of various UV scenarios to the ALP EFT. We have checked that the invariants indeed vanish if the UV completion features an exact PQ symmetry, i.e. shift symmetry, and have shown explicitly that the invariants will be proportional to the spurion of the shift symmetry breaking if such effects are present in the UV. We have also illustrated the collective aspect of the shift symmetry by considering scenarios that only make the invariants featuring both up- and down-type couplings non-vanishing.

We have shown that there exists a close connection between CP violation and shift symmetry at the leading order in the ALP EFT: all but one order parameters for the axion shift symmetry are CP-odd. The numbers in this relation can be explained by considering the field redefinition that allows to remove the shift of the ALP in the EFT. The field redefinition relies on a non-vanishing renormalisable SM Yukawa coupling, setting the number of constraints that have to be imposed.

Furthermore, we emphasised that the collective aspects of the invariants disappear when a non-linear realisation of the electroweak symmetry is considered and in the low-energy EFT, where all heavy particles of the SM are integrated out. Nevertheless, matching the low-energy theory, which captures both a linearly and non-linearly realised EW symmetry, to a UV completion with a linearly realised EW symmetry, we were able to show that the extra constraints implied by the linear realisation are stable under the RG flow in the IR. This allowed us to study constraints on the dimension-5 Wilson coefficients at low energy experiments like atomic EDMs with the constructed invariants. Furthermore, the flavour invariants allowed us to derive sum rules from the contribution of the ALP EFT to the running of the SMEFT Wilson coefficients.

Finally, we have extended the discussion to the non-perturbative breaking of the PQ symmetry induced by the coupling of the axions to gluons. We have identified the corresponding order parameter, which captures the mixed anomaly between the PQ and the $SU(3)_c$ symmetry, whenever a PQ symmetry exists at the classical level. We have shown that the additional order parameter does not run at 1-loop.

The results can be extended in several ways. We could connect the results to more CP-odd observables, which give strong constraints on new physics, due to the majority of the order parameters being CP-odd. It could also be interesting to study the collective nature of the order parameters at the level of observables and to further study the interplay between the flavourful axion couplings studied here, shift-breaking bosonic couplings of the axion and the axion mass. Lastly, it could also be interesting to compute the RG running below the EW scale at the next loop order to study to which precision the matching conditions to a linear realisation of the electroweak symmetry are preserved by the RG flow. Finite threshold corrections arising during the matching procedure at loop-level could also be included.

In the second third of Part II, we have studied how the shift-breaking effects in ALP EFTs above and below the electroweak scale can be captured beyond the leading interactions at dimension 5. To this end we have computed the Hilbert series of an ALP EFT with and without a shift symmetry above and below the EW scale. The Hilbert series allows us to perform the counting of the effective operators with full flavour dependence N_f, split into their transformation under CP and with and without lepton and baryon number conservation, which we have performed up to mass dimension 15. Using this information we have constructed operator bases for the ALP EFTs with and without a shift symmetry and above and below the EW scale up to mass dimension 8. Furthermore, we have constructed the invariants capturing the sources of CP violation of the leading order effective interactions.

The Hilbert series takes on a special form, which we call the PQ-breaking isolation condition, stating that beyond mass dimension 5 the operators describing shift-breaking couplings of the ALP to the SM are clearly isolated from the shift-preserving couplings. This is in stark contrast to what happens at dimension 5, where the EOM redundancy, relating the derivatively coupled operators with fermions to the ALP-Yukawa couplings, mixes the two sector of the EFT. The PQ-breaking isolation condition implies that no other such EOM redundancies exist at higher orders at least up to dimension 15, that we have checked. This means that at higher order only the effects of the EOM redundancy at dimension 5 on other higher-dimensional operators has to be tracked. We construct the relations on the higher-dimensional Wilson coefficient explicitly up to dimension 8, where also field redefinitions on SMEFT operators have to be taken into account, which a priori seem to be independent of the discussion in the ALP EFT. As an application of our operator basis, we derive positivity bounds on the dimension-8 Wilson coefficients in the ALP EFT above the EW scale.

The work could be extended as follows. First, we could study how the how the higher-dimensional shift-symmetric operators influence the phenomenology of ALPs. Since at dimension 5 the ALP already receives couplings to all SM particles except the Higgs, and at dimension 7 the ALP is coupled to all SM particles, we do not expect large corrections. The only exception could be specific channels which do not get a contribution in the EFT at lower mass order or which rely on intermediate particles from the SM implying that their amplitudes do not grow (as fast) with energy as a pure contact interaction. We could also study the interplay of shift-symmetric and shift-breaking operators if the scale of explicit PQ-breaking is not much larger than the scale of spontaneous breaking. In regards to low-energy experiments, our complete basis for the LEFT extended with an ALP should prove helpful to perform analyses beyond the leading order (c.f. for instance Ref. [189, 212]). Finally, with a complete basis one could extend the efforts of Refs. [212, 213, 286] and calculate the renormalisation group equations of operators of higher mass dimension and their contributions to the renormalisation group equations of operators at dimension 5. For these computations it would be helpful to construct a Green's basis, which we will do in an upcoming publication by computing the Hilbert series of the EFT keeping all EOM redundancies with the package `CHINCHILLA`, mentioned in Chaps. 3 and 7.

In the last third of Part II, we have considered new sources of CP violation in the UV in the presence of a small instanton background, which can destroy the axion solution to the strong CP problem by shifting the minimum of the axion potential.

To make the study independent of a specific UV model that provides the new sources of CP violation, we have parameterised the sources by CP-odd SMEFT operators. To capture the physical flavour-invariant sources of CP violation in those SMEFT operators, we have derived a new complete set of determinant-like flavour invariants, featuring the strong CP angle θ, which necessarily appears in instanton computations. The instanton computations were performed in the 1-instanton approximation, for which we have assumed that the strong coupling is large but still perturbative.

Because physical observables should be independent of a choice of basis, in particular a choice of flavour basis, the flavourful couplings should appear in the form of flavour invariants. Keeping all flavourful couplings generic in the instanton computations, the results of the path integral computation indeed depends on the determinant-like flavour invariants constructed earlier for all SMEFT operators. The old basis in terms of single-trace flavour invariants of Ref. [103], is less suited to perform these computations, which is obvious when the basis of determinant-like flavour invariants is projected on the trace basis: the trace invariants appear in complicated rational functions of polynomials. We have shown this explicitly for different examples.

Furthermore, the determinant-like invariants allow for a systematisation of the instanton computations. The structure of the invariants implies selection rules on which kind of operators can appear at the leading order in the instanton calculation since they determine the number of Yukawa couplings and loop factors. We have also shown that rephasing invariant operators cannot contribute only via fermion zero modes which usually give the dominant contribution. We showed, for instance, how to read off the additional loop suppression expected from the semi-leptonic operator $\mathcal{O}_{\text{lequ}}^{(1)}$ directly from the invariant. In addition, the flavour invariants allow to easily impose different flavour scenarios on all couplings in the theory. To this end, we have explicitly studied an anarchic, Froggatt–Nielsen, and minimally flavour-violating scenario. After also fixing the mechanism that enhances the effects of the small instantons in the UV, the experimental bound on $\overline{\theta}$ from the neutron EDM can be used to set bounds on the scale of new physics as a function of the scale where the small instantons arise. Comparing the operators $\mathcal{O}_{\text{quqd}}^{(1)}$ and $\mathcal{O}_{\text{dG}}$ in the product gauge group scenario, we find a similar bound of $\Lambda_{\not{CP}} \gtrsim 10^6\,\Lambda_{\text{SI}}$ for the MFV scenario, while for the anarchic scenario we obtain a limit of $\Lambda_{\not{CP}} \gtrsim 10^{11}\,\Lambda_{\text{SI}}$ for $\mathcal{O}_{\text{quqd}}^{(1)}$ and $\Lambda_{\not{CP}} \gtrsim 10^8\,\Lambda_{\text{SI}}$ for $\mathcal{O}_{\text{dG}}$, where we always assume that the contribution to $\overline{\theta}$ is entirely due to the effect of the small instantons.

The cancellation of divergences appearing in the loop integrals can be used as a non-trivial cross-check of our calculations. The divergences in the correlation functions are cancelled by including the counterterms of the SMEFT in a Green's basis. This cancellation has been explicitly shown for the semi-leptonic operator $\mathcal{O}_{\text{lequ}}^{(1)}$ to obtain a divergence-free result that is then used for the phenomenological study.

This work can be extended in several directions. The most immediate extension would be to perform a computation of the leading effect of all operators in the SMEFT to θ_{ind}, explicitly verifying the appearance of all other constructed invariants. In addition, including higher orders in the Yukawa couplings could be interesting to see the higher order invariants of the already considered operators arise. Another generalisation could be the inclusion of higher order effects in the EFT power counting (e.g. the double insertions of dimension-6 SMEFT operators or a single insertion of dimension-8 SMEFT operators), which would lead to new invariant structures with respect to the ones considered here. While we estimated that the higher order effects in the EFT are suppressed in the case of the double insertion of $\mathcal{O}_{\text{quqd}}^{(1)}$ in Appendix 8.A.1, it would still be interesting to perform such a study explicitly to understand the size of the corrections when all numerical factors are correctly taken into account.

Furthermore, here we have only considered the corrections to the minimum of the axion potential. In a future publication, we will also address the question how the small instanton scenarios considered here can also generate other shift-breaking operators of the axion like a mass term or even shift symmetry-breaking couplings to other SM fields. Here, the order parameters constructed in Chap. 6 could prove useful to check if the generated effective couplings indeed break the shift symmetry.

* * *

To close off this thesis, we want to return to the questions posed in the introduction. We have shown that flavour invariants are extremely useful tools in many situations in the presence of flavourful couplings. In particular, flavour invariants can be constructed to capture the necessary and sufficient conditions for CP conservation in a flavour-basis invariant way. To this end we have shown, how to construct the flavour invariants of the νSM and νSMEFT in Chaps. 3 and 4, how to build a complete set of CP-odd flavour invariants more suitable for instanton computations in Chap. 8 and we have constructed a complete set of CP-odd trace invariants for the ALP EFTs in Chap. 7. We have developed a graph-based algorithm that proved to be helpful for the brute-force construction of the invariants in the νSM but also for the systematic construction of the flavour invariants of the νSMEFT, where many flavourful couplings are present at the same time. This answers the questions of how the CP-odd invariants of commonly used EFTs look like and how to construct a basis for them suitable for computations.

In Chap. 6, we have shown that flavour invariants can also be useful in other contexts to describe the other aspects of symmetry breaking, in our case the ALP shift symmetry. To this end, we have presented how to disentangle the shift-preserving and shift-breaking interactions in ALP EFTs by using flavour invariants, that make it possible to properly implement the power countings of the shift-preserving and shift-breaking sector of the EFT. Besides this, the main advantage of the invariants is that they explicitly illustrate several features of shift symmetry, like its collectiveness due to the $SU(2)$ gauge structure of the EFT, the number of independent constraints that have to be imposed and its close connection to CP violation. We have also answered the question of how the relations imposing shift symmetry in the EFT can be generalised to higher orders in the EFT expansion in Chap. 7.

The last question we posed in the introduction was if the EFT flavour invariants are really the fundamental objects that appear in computations without further suppressions or enhancements by other flavourful but flavour-invariant objects. In the instanton computations, where we have calculated the shift of the axion potential minimum induced by CP-violating SMEFT operators, we have shown explicitly that this is indeed the case. Note however, that this was strongly basis-dependent. Had we used a basis of single-trace flavour invariants, the result would have been a complicated rational function of polynomials as we showed in Sec. 8.2.1. Because the computations do not care about the chosen set of basis invariants, it is likely that invariants outside of the chosen basis will be generated that subsequently have to be projected back onto the original basis. Here, the numerical algorithm presented in Chap. 3 could prove useful to find all the relations that relate an invariant from outside of the basis to the basis invariants. What remains to show is that the same is also true for perturbative computations of CP-odd observables. If the invariants there come suppressed with other flavourful but flavour-invariant objects, it could again be due to a bad choice of an invariant basis or simply because the EFT invariants should indeed not be interpreted as a quantitative measure of CP violation. Either way, the invariants still qualitatively capture fundamental properties of the EFT, like the violation of CP or shift symmetry, and are hence useful tools to organise computations.

A lot of exciting experimental work lies ahead of us in the upcoming years and decades improving the precision of our knowledge of several corners of the SM. The high-luminosity upgrade of the LHC, for instance, will give us unprecedented precision in particular in the Higgs and electroweak sector with measurements starting in 2029. This will improve our reach for BSM physics in those areas significantly. Furthermore, the ever-increasing precision in neutrino experiments will soon allow us to pin down the value of neutrino masses and the existence and size of CP violation in the neutrino sector. This is particularly exciting as both results would be a definite sign for new physics guiding us towards a UV completion that can resolve the problem of neutrino masses in the SM and potentially can potentially also explain the baryon asymmetry through leptogenesis. Other thrilling experiments are also proposed, further improving sensitivity to CP-violating new physics. For instance, a storage ring for protons was proposed to measure the proton EDM, improving the reach for new sources of CP violation by four orders of magnitude [364]. Another exciting development are small tabletop experiments, which despite their smallness have an incredible constraining power for BSM physics. One particularly interesting example is the ACME experiment, measuring the electric dipole moment of the electron. The upcoming results of the third stage of the experiment will push the open window left for CP-violating BSM physics hiding below current limits even closer to the SM background. Lastly, many experiments are also looking for axions and ALPs. For instance, the ALPS experiment at DESY looks for ALPs with their coupling to photons by measuring if light can be shined through a wall by intermediately converting it into an ALP with magnetic fields [365].

Hence, many areas of well-motivated new physics will be probed in the next few decades. In this upcoming precision era of particle physics experiments, EFT tools will be indispensable in systematising, simplifying and improving the interpretability of these results. In particular, significant progress is made in the measurement of CP-violating observables in several directions. Here, the CP-odd flavour invariants developed in this thesis could help in efficiently interpreting the results of those experiments. Should an ALP be detected in any of the ongoing searches, one of its important properties that needs to be further investigated is its coupling to gluons and whether it has a shift symmetry, which could identify it as the QCD axion. Hence, pushing forward the understanding of the shift symmetry of ALPs in the EFT language is a vital step in properly interpreting possible future experimental results. Together, these EFT tools will hopefully make a contribution in bringing us a step closer to a more fundamental understanding of our Universe.

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