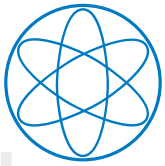
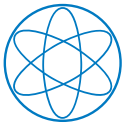


Dissertation

Discrete Groups in Model Building and the Definition of CP

Maximilian Fallbacher

Technische Universität München



Technische Universität München
Department Physik
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Dissertation

Discrete Groups in Model Building and the Definition of CP

Maximilian Karl Fallbacher

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Abstract

Discrete non-abelian flavour symmetries are attractive candidates for a solution to the flavour problem of the Standard Model. After an introduction to finite group theory and the flavour problem, conditions for such symmetries to be anomaly free are presented. In flavour models with discrete non-abelian symmetries, there are corrections to the kinetic terms of matter fields which change their mixing structure. The resulting effects on neutrino mixing are computed and shown to be non-negligible. In order to build models in which a discrete group is obtained from the spontaneous breaking of a continuous group, the corresponding branching rules must be known. It is shown how to derive these rules for the decomposition of representations of the compact classical Lie groups into representations of arbitrary finite subgroups. Furthermore, the definition of proper physical CP transformations in the presence of discrete non-abelian symmetries is investigated in detail, and the connection of CP to class-inverting automorphisms is derived. It is thereby shown that some groups do not, in general, allow for the definition of a consistent CP transformation.

Zusammenfassung

Diskrete nichtabelsche Flavoursymmetrien sind attraktive Kandidaten für die Lösung des Flavourproblems des Standardmodells. Nach einer Einführung in die Theorie endlicher Gruppen und in das Flavourproblem werden Bedingungen dafür aufgestellt, dass solche Symmetrien anomaliefrei sind. In Flavourmodellen mit diskreten nichtabelschen Symmetrien treten Korrekturen zu den kinetischen Termen der Materiefelder auf, die deren Mischungsstruktur ändern. Die Auswirkungen der Korrekturen auf die Neutrinomischung werden berechnet und es wird gezeigt, dass diese nicht vernachlässigbar sind. Zur Aufstellung von Modellen, in denen eine diskrete Gruppe durch spontane Brechung einer kontinuierlichen Gruppe erzeugt wird, müssen die entsprechenden Verzweigungsregeln bekannt sein. Es wird gezeigt, wie diese Regeln für die Zerlegung von Darstellungen der kompakten klassischen Liegruppen in Darstellungen beliebiger endlicher Untergruppen berechnet werden können. Darüber hinaus wird die Definition von physikalischen CP-Transformationen in Modellen mit diskreten nichtabelschen Symmetrien detailliert untersucht und die Verbindung von CP zu klasseninvertierenden Automorphismen hergeleitet. Dabei wird gezeigt, dass es für einige Gruppen im Allgemeinen nicht möglich ist, eine konsistente CP-Transformation zu definieren.

Contents

I Introduction

The Standard Model of particle physics (SM) [7, 8] is undoubtedly one of the most successful models of physics ever conceived. In countless years of experiments, including run I of the Large Hadron Collider, physicists have been able to pin down the parameters of the SM ever more precisely without detecting any clear evidence for inconsistencies. On the experimental side, therefore, only the existence of neutrino masses, which can, however, easily be incorporated in an extension of the SM, the cosmological evidence for Dark Matter and the fact that gravity is not described by the SM point towards the necessity for a more fundamental theory.

Independently of these successes in describing experimental results and of the already mentioned deficiencies, there are several theoretical reasons rendering a more fundamental theory than the SM desirable. A very prominent role amongst them plays the hierarchy problem, i.e. the question why the electroweak scale is suppressed by many orders of magnitude against the Planck scale. A second and certainly not less pressing issue of the Standard Model is the so-called flavour problem. Even though the SM provides a framework that can be used to fit experimental results, it requires about 20 input parameters to do so. These parameters are not predicted by the theory itself but must be set by hand in order to accommodate experimental results. Especially in the flavour sector, i.e. the sector responsible for the masses of matter particles, this abundance of input parameters seems an issue. Moreover, the required coupling values are not, as one might expect, clustered close to unity but span many orders of magnitude. At the same time, there seems to be a pattern behind the mixing angles connecting the different generations of quarks and leptons, respectively. In addition, the so-called CP symmetry is broken in Nature, i.e. replacing particles with their anti-particles and simultaneously right-handed with left-handed particles is not a symmetry. Although this can again easily be parametrised by the explicitly CP violating Dirac CP phase of the quark sector, the SM does not provide any further insight into this breaking.

Of course, one would like to explain these observations on a fundamental level and not merely parametrise them. So-called flavour symmetries are a possible avenue one can pursue to this end. In this framework, it is assumed that a symmetry relates the different generations of matter fields at high energies. At some lower energy scale, the symmetry is spontaneously broken, thereby generating a structure for the mass terms. The difficulty is to find a symmetry that generates the desired mass, mixing and CP violation patterns in a natural fashion. Moreover, first-order calculations are often insufficient since higher-order effects can spoil the leading-order predictions. The estimation of these corrections, however, can be computationally very demanding.

Amongst the different types of symmetries available for this purpose to model builders, discrete non-abelian symmetries are arguably the most promising alternative. Since they are non-abelian, they are able to generate non-trivial mixing patterns. Furthermore, they do not suffer from issues connected to Goldstone bosons that would be unavoidable in the spontaneous breaking of global continuous symmetries. It is the purpose of this work to present progress concerning several aspects of model building with discrete non-abelian symmetries and to aid the construction of such models of physics beyond the SM.

For the discussion of the physical implications of discrete symmetries, a sound knowledge of finite group theory is indispensable. Therefore, in Chapter II, some basic information on the theory of finite groups is compiled. Besides some general definitions and theorems, the notion of Clebsch–Gordan coefficients is particularly important because these coefficients are needed for the construction of Lagrangians. However, Clebsch–Gordan coefficients are not uniquely determined; hence, the resultant ambiguities in general and the corresponding implications for model building in particular are explained in some detail.

In Chapter III, a brief introduction to the flavour problem of the Standard Model is given. An important point in the discussion of the SM flavour sector is the introduction of the so-called CKM and PMNS mixing matrices of the quark and neutrino sector, respectively. Particular care is exercised with respect to their phase and sign ambiguities, which are important for the later discussion of kinetic term corrections. Subsequently, the aforementioned discrete non-abelian flavour symmetries are advertised as a means to explain the observed flavour structure. Moreover, a neutrino flavour model based on the tetrahedral group A_4, also called alternating group on four letters, is presented. This model was originally proposed by Altarelli and Feruglio [9, 10]. It is ideally suited to understand the salient features of flavour models with discrete non-abelian symmetries and is used also as an example model in the later discussion of the kinetic term corrections. In the conclusion of the chapter, some of the well-known criticism towards such models is compiled and commented on.

As is well known, a symmetry of a classical Lagrangian or classical action is not necessarily a symmetry of the corresponding quantum theory. In such a case, the symmetry is said to be anomalous. This does not only occur for continuous but also for discrete symmetries. Conditions for discrete groups to be free of anomalies are thus derived in Chapter IV. In particular, it is shown that the path integral measure transforms in a proper one-dimensional representation of the group. From this observation, a series of interesting results follows. For example, discrete groups are less prone to anomalies in combination with $\mathrm{SO}(N)$ or exceptional gauge groups than in combination with $\mathrm{SU}(N)$.

Model building with discrete flavour symmetries, like the aforementioned A_4 model, usually proceeds in the framework of effective field theories. Thus, one has to consider higher-order corrections to the lowest-order results that are computed first. In particular, there are corrections to the kinetic terms of matter fields, which can change their normalisations and induce a mixing. As shown in Chapter V, these corrections can have profound implications for model predictions such as flavour mixing; however, these effects have often been neglected in the literature. To facilitate the estimation of their impact, analytical formulas are derived which depend only on the naive masses and mixing parameters computed without taking into account the corrections. These formulas are also incorporated into a publicly available Mathematica [11] package. Note that, for simplicity, the discussion is presented using a supersymmetric terminology, in which the corrections are called Kähler corrections, although such effects are present independently of supersymmetry. As is shown using the A_4 model and another model based on the group T′, the effects of kinetic term

corrections on the mixing angles can be large. In addition, the impact of Kähler corrections in supersymmetric models on the vacuum alignment and on flavour changing neutral currents is briefly described.

Although discrete symmetries are very useful for model building, there are various reasons to assume that they are not fundamental. For example, as all global symmetries, they are conjectured to be violated badly by gravitational effects, which thereby render them ineffective [12, 13]. One possible solution is to obtain a discrete group from spontaneous breaking of a continuous gauge group. In order to do so, knowledge of the branching rules of representations of the gauge group into representations of the discrete subgroup is required. In particular, only representations of the gauge group whose decomposition contains at least one trivial singlet of the discrete group can be used for the breaking. A procedure for the computation of these branching rules is presented in Chapter VI. The resulting routines are furthermore implemented in a publicly available MATHEMATICA package. Indeed, one can use the package to compute general branching rules for some finite groups which are popular in model building. Some examples of such decomposition rules are given and their implications discussed.

One of the least understood phenomena of particle physics is the violation of the combination of charge conjugation and parity transformation denoted by CP. Although in the context of the Standard Model it is clear how this transformation acts on the fields, this is more intricate if discrete symmetries are present. Building on work by Grimus and Rebelo [14], Holthausen, Lindner and Schmidt [15] and Feruglio, Hagedorn and Ziegler [16], in Chapter VII, the interplay of discrete (flavour) symmetries and CP is investigated in detail. After discussing the CP transformations of Quantum Electrodynamics and of the SM, the results of the aforementioned publications are reviewed. As it turns out, their criteria are insufficient to obtain proper physical CP transformations if discrete symmetries are present. The correct group theoretical conditions are presented, connecting CP transformations to so-called class-inverting automorphisms, and some mathematical tools for the necessary computations are introduced. The resulting constraints on the availability of CP transformations are discussed. In particular, it is shown that there are groups which for generic settings do not allow CP consistently to be defined. This is also seen in a toy model based on the group $\Delta(27)$. Furthermore, in a modification of this model, spontaneous CP violation with group theoretical, i.e. calculable, phases is achieved. Another model with CP violation due to calculable phases is the three Higgs doublet model by Branco, Gerard and Grimus [17], where this effect is called geometrical CP violation. The model is briefly reviewed and some misconceptions concerning this type of CP violation are corrected. Subsequently, the usability of generalised CP transformations as solutions to the strong CP problem is discussed. Moreover, the spontaneous breaking of discrete groups and of CP transformations is re-considered with regard to the group theoretical structure of CP. Finally, some more fundamental considerations are taken up concerning the connection of CP to the inversion of all quantum numbers. After concluding this part, three publications by other authors related to generalised CP transformations are commented on.

After the main conclusion, some appendices contain material omitted in the main text. In Appendix A, notations and bases for some frequently used groups as well as some additional mathematical theorems and proofs can be found. In the subsequent Appendix B, analytical formulas for kinetic term corrections to tri-bi-maximal mixing are shown. Some of the GAP codes used to compute the results of Chapter VII are presented in Appendix C. Finally, a list with the numbers of distinct CP transformations for finite groups up to order 100 can be found in Appendix D.

It should be noted that, although flavour symmetries are mostly chosen as examples, almost all results obtained here are independent of the precise purpose for which the discrete non-abelian symmetries are employed. For example, the anomaly computations in Chapter IV and the discussion of CP transformations in Chapter VII are completely independent of whether the discrete non-abelian symmetry is used to explain the flavour structure of the Standard Model or for some other purpose.

Some of the results presented here have already been communicated in the following publications:

[1] M.-C. Chen, M. Fallbacher, M. Ratz and C. Staudt, 'On predictions from spontaneously broken flavor symmetries', *Phys. Lett.* B **718** (2012), 516–521, arXiv: 1208.2947 [hep-ph], [inSPIRE].

[2] M.-C. Chen, M. Fallbacher, Y. Omura, M. Ratz and C. Staudt, 'Predictivity of models with spontaneously broken non-Abelian discrete flavor symmetries', *Nucl. Phys.* B **873** (2013), 343–371, arXiv: 1302.5576 [hep-ph], [inSPIRE].

[3] M.-C. Chen, M. Fallbacher, K. T. Mahanthappa, M. Ratz and A. Trautner, 'CP violation from finite groups', *Nucl. Phys.* B **883** (2014), 267–305, arXiv: 1402.0507 [hep-ph], [inSPIRE].

[4] M. Fallbacher and A. Trautner, 'Symmetries of symmetries and geometrical CP violation', *Nucl. Phys.* B **894** (2015), 136–160, arXiv: 1502.01829 [hep-ph], [inSPIRE].

[5] M.-C. Chen, M. Fallbacher, M. Ratz, A. Trautner and P. K. S. Vaudrevange, 'Anomaly-safe discrete groups', *Phys. Lett.* B **747** (2015), 22–26, arXiv: 1504.03470 [hep-ph], [inSPIRE].

[6] M. Fallbacher, 'Breaking classical Lie groups to finite subgroups – an automated approach', *Nucl. Phys.* B **898** (2015), 229–247, arXiv: 1506.03677 [hep-th], [inSPIRE].

II Group theory

In many parts of this text, heavy use is made of finite group theory. For example, in order to build models with discrete symmetry groups as reviewed in Chapter III and to interpret their results as done for a special case in Chapter V, one has to understand the construction of invariant Lagrangians using Clebsch–Gordan coefficients. Moreover, many properties of such models like their behaviour with respect to CP, see Chapter VII, or with respect to anomalies, see Chapter IV, depend on the relations imposed on them by the symmetries, which in turn are determined by the structure of the symmetry groups. Only with a good knowledge of group theory these discussions can be led. Therefore, some basic notions of group theory are reviewed in the present chapter, including the concepts of representations, characters, group automorphisms, tensor products of representations and Clebsch–Gordan coefficients. Moreover, some notation used later on is introduced.

Since most of the material presented in this chapter is well known, the corresponding references are to textbooks rather than to original research contributions. Moreover, proofs for most of the theorems stated below are not reproduced but can be found in the cited sources. For more information on the topic, cf. any book on group and representation theory, e.g. [18, 19].

First, the concepts of groups and of group homomorphisms are introduced. Since most often symmetry groups of physical models are direct or semi-direct product groups, e.g. $G_{SM} = SU(3)_C \times SU(2)_L \times U(1)_Y$, these notions are explained in the second section. The most important topic in group theory for physics is probably representation theory, whose basic concepts are presented in Section II.3. A closely related and very powerful computational tool are group characters, which are introduced subsequently. Section II.5 then gives the definition of real and pseudo-real representations.

Whereas everything up to this point would also be of use to non-physicists, the last two sections are more focused on the physics application. Hence, they might also be interesting for readers who are otherwise proficient in group theory.

In Section II.6, the concept of tensor products of representations and Clebsch–Gordan coefficients is explained. Since this topic is absolutely crucial for model building, the discussion is rather detailed. In particular, the ambiguities that arise in the definition of Clebsch–Gordan coefficients are clarified. These ambiguities are often neglected but are very important when discussing the CP properties of a theory. Another topic that is usually glossed over concerns the associativity of the tensor product. Due to the way model builders usually write down Lagrangians, an associated subtlety can lead to ambiguities when specifying a model.

Details on some finite groups which are used extensively in this text are collected in Section A.1. Information on other finite groups of small orders can easily be obtained using the SmallGroups library of the group theory software GAP [20].

II.1 Groups and group homomorphisms

For completeness, let us start with some very basic definitions.

Definition 1 (Group). *A group G is a set, also called G, together with a closed binary operation most often called multiplication,*

$$\begin{array}{rccl} \star: & G\times G & \to & G\,, \\ & (a,\,b) & \mapsto & a\star b\,, \end{array} \tag{1.1}$$

which is associative, $a\star(b\star c)=(a\star b)\star c$. Moreover, there has to be an identity element $e\in G$ such that $e\star a=a$ for all $a\in G$, and for each element $a\in G$ there has to be an inverse $a^{-1}\in G$ with $a^{-1}\star a=e$. A group G is called abelian if $a\star b=b\star a$ for all $a,\,b\in G$ and non-abelian otherwise. A subgroup H of G, $H\leq G$, is a subset of G that is closed under group multiplication and inversion.

Note that the multiplication symbol $\star$ is omitted henceforth; the product of two group elements a and b is just denoted by ab if there is no danger of confusion.

Groups can be finite sets, in which case the number of elements $|G|$ of G is called the order of G, or infinite. This work restricts the notion of group to compact topological groups, i.e. groups which are, with respect to their natural topology, compact, and whose binary operation as well as inverse map are continuous. The focus is set on finite groups and compact Lie groups.

Definition 2 (Lie group). *A Lie group G is a differentiable manifold with a group structure such that group multiplication and inverse map are smooth.*

As a special case, the general linear group of a vector space shall be defined because it is needed for the definition of group representations.

Definition 3 (General linear group). *The general linear group $\mathrm{GL}(V)$ of a vector space V is the group of all automorphisms of V, i.e. of all bijective linear maps on V. If V is finite dimensional, $\dim V=n<\infty$, $\mathrm{GL}(V)$ is isomorphic to the group $\mathrm{GL}(n,K)$ of all invertible $n\times n$-matrices over the base field K.*

The most important type of maps between groups are maps that are compatible with the group structure, so-called group homomorphisms.

Definition 4 (Group homomorphism). *Given two groups G with operation $\star$ and H with operation $*$, respectively, any map*

$$\begin{array}{rccl} \varphi: & G & \to & H \end{array} \tag{1.2}$$

with $\varphi(a\star b)=\varphi(a)*\varphi(b)$ for all $a,\,b\in G$ is called a group homomorphism. If φ is a bijection and $G=H$, φ is called an automorphism.

Definition 5 (Automorphism group). *The automorphisms of a group G form another group, the automorphism group $\mathrm{Aut}(G)$.*

Definition 6 (Conjugator automorphism and inner automorphism group)**.** *For each group element g, the associated conjugation map* $\mathrm{conj}(g)$ *with* $\mathrm{conj}(g)(h) := ghg^{-1}$ *for all* $h \in G$ *is an automorphism. These automorphisms are called inner automorphisms. They form the group of inner automorphisms* $\mathrm{Inn}(G) \leq \mathrm{Aut}(G)$*.*

Definition 7 (Conjugacy class)**.** *Being related by an inner automorphism defines an equivalence relation on the set of group elements. The equivalence classes of this relation are called conjugacy classes.*

Definition 8 (Normal subgroup)**.** *A subgroup* $N \leq G$ *that is invariant under all inner automorphisms is called normal subgroup* $N \trianglelefteq G$*.*

Definition 9 (Simple group)**.** *A group G is simple if and only if it has no non-trivial normal subgroup, i.e. if its only normal subgroups are G itself and the trivial group.*

Definition 10 (Centre)**.** *The centre* $Z(G)$ *of a group G is the normal subgroup of G containing all group elements that commute with every other group element.*

Definition 11 (Quotient group)**.** *The equivalence classes* G/N*, where N is a normal subgroup of G, define a group, the so-called quotient group of G by N. The canonical projection*

$$\begin{array}{rccl} p: & G & \to & G/N, \\ & g & \mapsto & [g] \end{array} \tag{1.3}$$

is the surjective group homomorphism sending each element of G to its equivalence class in G/N*.*

Definition 12 (Outer automorphism group)**.** *The inner automorphisms form a normal subgroup of the automorphism group. The corresponding quotient group* $\mathrm{Out}(G) := \mathrm{Aut}(G)/\mathrm{Inn}(G)$ *is called outer automorphism group.*

Note that outer automorphisms, i.e. the elements of the outer automorphism group, are not automorphisms but equivalence classes of automorphisms.

Definition 13 (Commutator subgroup and Abelianisation [21])**.** *The commutator or derived subgroup* $[G, G]$ *(or* G'*) is the subgroup of G generated by all commutator elements of G,*

$$[G, G] := \left\langle \{g \in G \,|\, g = aba^{-1}b^{-1},\, a \in G,\, b \in G\} \right\rangle. \tag{1.4}$$

It is a normal subgroup of G because commutators are invariant under any automorphism of G. The corresponding quotient group $A(G) := G/[G, G]$ *is abelian and called Abelianisation of G.*

Definition 14 (Perfect group)**.** *A group G is called perfect if and only if it equals its own commutator subgroup. This is the same as saying that its Abelianisation* $A(G)$ *is trivial.*

Theorem 1 (Non-abelian simple groups are perfect)**.** *A non-abelian simple group G is perfect.*

This can be seen by noting that the commutator subgroup is a normal subgroup. Thus, the commutator subgroup of a simple group can only be the group itself, in which case the group is abelian, or the trivial group, in which case the group is perfect.

II.2 Direct and semi-direct product of groups

Definition 15 (Direct product [19]). *A group G is the inner direct product of subgroups A_i,*

$$G = A_1 \times A_2 \times \cdots \times A_n \,, \tag{2.1}$$

if and only if the following conditions are fulfilled:

(i) *all A_i are normal subgroups or, equivalently, they all commute;*

(ii) *the set product $\prod_i A_i$ generates G;*

(iii) *each A_i intersects trivially the subgroup generated by the $A_{j\neq i}$ or, equivalently, each element $g \in G$ has a unique decomposition into $\prod_i a_i$ with $a_i \in A_i$.*

The direct product of groups A_i is again a group G with the multiplication

$$(a_1, \dots, a_n)(b_1, \dots, b_n) \coloneqq (a_1 b_1, \dots, a_n b_n) \,. \tag{2.2}$$

The resulting group G fulfils the three conditions above.

The concept of direct product groups can be used completely to classify the finite abelian groups.

Theorem 2 (Fundamental theorem on finite abelian groups [22]). *Any finite abelian group G is isomorphic to the direct product of cyclic groups of orders which are powers $n^{i,j}$ of prime numbers p_i,*

$$G \cong \bigtimes_{i,j} \mathbb{Z}_{p_i^{n^{i,j}}} \,. \tag{2.3}$$

A generalisation of the direct product of two groups is their semi-direct product.

Definition 16 (Semi-direct product [19]). *A group G is the semi-direct product of two subgroups N and H,*

$$G = N \rtimes H \,, \tag{2.4}$$

if and only if the following conditions are fulfilled:

(i) *N is a normal subgroup;*

(ii) *the set product NH generates G;*

(iii) *$N \cap H = \{e\}$ or, equivalently, each element $g \in G$ has a unique decomposition into a product nh with $n \in N$ and $h \in H$.*

On the other hand, the Cartesian product of sets $N \times H$ can be made into the semi-direct product group $N \rtimes H$ by the multiplication

$$(n, h)(n', h') \coloneqq (n\varphi(h)(n'), hh') \tag{2.5}$$

where φ is any group homomorphism from H to the automorphism group of N.

In the special case $\varphi \equiv \mathrm{id}$ the semi-direct product becomes the direct product.

II.3 Representations

Group representations are a particular form of group homomorphisms.

Definition 17 (Group representation)**.** *A continuous homomorphism $\boldsymbol{R}$ from a group G to the general linear group $\mathrm{GL}(V)$ of a vector space V*

$$\boldsymbol{R}: \quad G \quad \to \quad \mathrm{GL}(V) \tag{3.1}$$

is called (linear) representation. The dimension (or degree) of a representation is the same as the dimension of its representation space, $\dim \boldsymbol{R} := \dim V$. If the representation homomorphism is an injection, the representation is called faithful. A subrepresentation is a proper, non-trivial subspace W of V such that W is invariant under $\boldsymbol{R}$. If V has no such subspace, $\boldsymbol{R}$ is called an irreducible representation. A representation is unitary if $\boldsymbol{R}(g)$ is a unitary operator for all $g \in G$, i.e. if it preserves the inner product on V.

Only finite-dimensional representations over the base field $\mathbb{C}$ are considered hereafter. The specification of a representation $\boldsymbol{R}$ is, of course, incomplete without the specification of the corresponding representation space V. However, the representation space is usually suppressed in the notation. In these cases it is understood that the space is $V = \mathbb{C}^{\dim \boldsymbol{R}}$.

For finite groups, the dimension of an irreducible representation divides the order of the group [18]. The number of inequivalent irreducible representations of a finite group is equal to the number of conjugacy classes, and the sum of the squares of the dimensions of all inequivalent irreducible representations $\boldsymbol{R}_i$ equals the order of the group [19],

$$\sum_i (\dim \boldsymbol{R}_i)^2 = |G| \,. \tag{3.2}$$

For finite-dimensional representation spaces V over the field K the term representation is also used for a specific matrix realisation

$$\begin{aligned} \rho_{\boldsymbol{R}}: \quad G \quad &\to \quad \mathrm{GL}(n, K) \,, \\ g \quad &\mapsto \quad \rho_{\boldsymbol{R}}(g) \,. \end{aligned} \tag{3.3}$$

Hence, representation can refer, interchangeably, to either the representation space, the map into the general linear group of this space or the map into the invertible matrices for some choice of basis on the representation space.

Definition 18 (Complex conjugate representation)**.** *Given a representation $\boldsymbol{R}$ on V one can define the complex conjugate representation $\overline{\boldsymbol{R}}$ on the complex conjugate vector space $\overline{V}$ by*

$$\overline{\boldsymbol{R}}: \quad G \quad \to \quad \mathrm{GL}(\overline{V}) \tag{3.4}$$

with $\overline{\boldsymbol{R}}(g)(v^*) := (\boldsymbol{R}(g)(v))^*$ for all $v^* \in \overline{V}$.

The irreducible representations of abelian groups have a very elementary structure.

Theorem 3 (Irreducible representations of abelian groups [19])**.** *All irreducible representations of abelian groups are one-dimensional.*

Given two, not necessarily distinct, representations it is possible to obtain a representation on the direct sum and on the tensor product of the respective vector spaces.

Definition 19 (Direct sum and tensor product of representations [19]). *The direct sum of two representations $\boldsymbol{R}$ and $\boldsymbol{R}'$ of G on V and W, respectively, is the representation on $V \oplus W$ defined by*

$$\begin{aligned} \boldsymbol{R} \oplus \boldsymbol{R}' : \quad G &\to \mathrm{GL}(V \oplus W)\,, \\ g &\mapsto (\boldsymbol{R} \oplus \boldsymbol{R}')(g) \end{aligned} \tag{3.5}$$

where $(\boldsymbol{R} \oplus \boldsymbol{R}')(g)(v \oplus w) := \boldsymbol{R}(g)(v) \oplus \boldsymbol{R}'(g)(w)$.

One can also define a representation on the tensor product space $V \otimes W$ by

$$\begin{aligned} \boldsymbol{R} \otimes \boldsymbol{R}' : \quad G &\to \mathrm{GL}(V \otimes W)\,, \\ g &\mapsto (\boldsymbol{R} \otimes \boldsymbol{R}')(g) \end{aligned} \tag{3.6}$$

with $(\boldsymbol{R} \otimes \boldsymbol{R}')(g)(v \otimes w) := \boldsymbol{R}(g)(v) \otimes \boldsymbol{R}'(g)(w)$.

Theorem 4 (Irreducible representations of direct product groups [19]). *Given two representations $\boldsymbol{R}$ on V of G_1 and $\boldsymbol{R}'$ on W of G_2, the tensor product representation*

$$\begin{aligned} \boldsymbol{R} \otimes \boldsymbol{R}' : \quad G_1 \times G_2 &\to \mathrm{GL}(V) \otimes \mathrm{GL}(W)\,, \\ (g_1, g_2) &\mapsto \boldsymbol{R}(g_1) \otimes \boldsymbol{R}'(g_2) \end{aligned} \tag{3.7}$$

with $(\boldsymbol{R}(g_1) \otimes \boldsymbol{R}'(g_2))(v \otimes w) := \boldsymbol{R}(g_1)(v) \otimes \boldsymbol{R}'(g_2)(w)$ is a representation of $G = G_1 \times G_2$. In fact, the irreducible representations of G are the representation obtained this way from all irreducible representations of G_1 and G_2.

Theorem 5 (Representations of quotient groups [21]). *The representations of a quotient group G/N are in bijective correspondence with the representations of G whose kernel contains N. The bijection is provided by the canonical projection and its pre-image, respectively. For compact groups the one-to-one correspondence is one of irreducible representations.*

To be more explicit, let $\boldsymbol{R}$ be a representation of G, $\boldsymbol{r}$ be a representation of G/N and p be the canonical projection of G onto G/N. If $\boldsymbol{R}$ is constant on N, the composition $\boldsymbol{R} \circ p^{-1}$ is well defined and a representation of G/N. Conversely, $\boldsymbol{r} \circ p$ is a representation of G which is constant on N. The fact that this is a bijection between irreducible representations in the case of compact G can easily be seen using group characters, which are introduced below in Section II.4. The proof is thus deferred to this section, see equation (4.5).

This theorem can be applied to the special case of the Abelianisation of a group.

Theorem 6 (One-dimensional representations and the Abelianisation [21]). *There is a one-to-one correspondence between the one-dimensional representations of a group G and the representations of its Abelianisation $A(G)$.*

The first direction is clear because $A(G)$ is abelian and, hence, has only one-dimensional irreducible representations, which lift to one-dimensional representations of G by Theorem 5. The second direction works out because all elements of G which are also contained in $[G, G]$ are sent to 1 by any one-dimensional representation as complex numbers commute. Thus, Theorem 5 can be applied again.

Maps between representation spaces should be compatible with the group action.

Definition 20 (Intertwiner). *A linear map φ between two representation spaces V with representation $\boldsymbol{R}$ and W with representation $\boldsymbol{R}'$ is called intertwiner if and only if it commutes with the group action,*

$$\varphi \circ \boldsymbol{R} = \boldsymbol{R}' \circ \varphi\,. \tag{3.8}$$

The intertwiners make up the vector space $\mathrm{Hom}_G(V, W)$. If the intertwiner φ is an automorphism, the two representations $\boldsymbol{R}$ and $\boldsymbol{R}'$ are called equivalent, $\boldsymbol{R} \cong \boldsymbol{R}'$.

This defines an equivalence relation on the set of all representations of a group. In particular, when referring to irreducible representations, usually the qualification 'inequivalent' is understood to avoid double-counting. Bold letters and, when referring to representations of a specific group, bold numbers denote henceforth equivalence classes of (mostly irreducible) representations. Specific matrix realisations thereof, i.e. the matrices that one obtains after choosing a certain fixed representation and a basis convention, are denoted by $\rho_{\boldsymbol{R}}$ for a representation in the equivalence class $\boldsymbol{R}$ of representations.

The fact that $\mathbb{C}$ is algebraically closed and has characteristic zero simplifies many discussions or is even a necessary condition. As a result of the assumptions made so far, the following theorems hold.

Theorem 7 (All representations are unitary [23])**.** *Every representation is equivalent to a unitary representation.*

Theorem 8 (Complete reducibility [23])**.** *Every representation is completely reducible, i.e. it is a direct sum of irreducible representations.*

Another important theorem for finite-dimensional representations, which basically follows directly from the definition of irreducibility, is Schur's lemma.

Theorem 9 (Schur's lemma [23])**.** *If φ is an intertwiner of two irreducible representation spaces V and W, then either*

(i) $\varphi \equiv 0$ or

(ii) φ is an isomorphism, i.e. the two representations are equivalent.

If φ is a self-intertwiner, i.e. $V = W$, then $\varphi = \lambda \,\mathrm{id}$ for some complex number λ.

It can also be shown that the matrix elements of finite-dimensional representations are, in a certain way, orthogonal to each other. The notation is adapted to the case of finite groups. The statement stays true for non-finite compact groups if the normalised summation over all group elements $\frac{1}{|G|}\sum_{g\in G}$ is replaced by an integration over the group with respect to the unimodular Haar measure.

Theorem 10 (Schur orthogonality [23])**.** *Let $\boldsymbol{R}_i$ be the irreducible representations of a finite group G. Then the matrix elements of these representations are orthogonal to each other,*

$$\frac{1}{|G|}\sum_{g\in G}\left[\rho_{\boldsymbol{R}_i}(g^{-1})\right]_{km}\left[\rho_{\boldsymbol{R}_j}(g)\right]_{nl} = \frac{1}{\dim \boldsymbol{R}_i}\,\delta_{ij}\,\delta_{kl}\,\delta_{mn}\,, \tag{3.9}$$

which can also be written for unitary representations as (please observe the change of indices on the left-hand side)

$$\frac{1}{|G|}\sum_{g\in G}\left[\rho_{\boldsymbol{R}_i}(g)^*\right]_{km}\left[\rho_{\boldsymbol{R}_j}(g)\right]_{ln} = \frac{1}{\dim \boldsymbol{R}_i}\,\delta_{ij}\,\delta_{kl}\,\delta_{mn}\,. \tag{3.10}$$

In both equations δ_{ij} is one if $\boldsymbol{R}_i \cong \boldsymbol{R}_j$ and zero otherwise.

II.4 Group characters

An important tool for group theory proofs and computations are group characters. Many results can be obtained using characters without resorting to a specific matrix realisation of a representation.

Let G be, as above, a compact topological group and consider its representations over the complex numbers.

Definition 21 (Group character [23]). *Given a representation $\boldsymbol{R}$ with matrix realisation $\rho_{\boldsymbol{R}}(g)$ its character is defined by*

$$\begin{aligned} \chi_{\boldsymbol{R}} : \; G &\to \mathbb{C}\,, \\ g &\mapsto \chi_{\boldsymbol{R}}(g) \coloneqq \operatorname{tr} \boldsymbol{R}(g) = \operatorname{tr} \rho_{\boldsymbol{R}}(g)\,, \end{aligned} \tag{4.1}$$

where the last equality is true for any matrix realisation because the trace is basis invariant. By the same argument, characters are class functions, i.e. they are constant on conjugacy classes, $\chi_{\boldsymbol{R}}(hgh^{-1}) = \chi_{\boldsymbol{R}}(g)$ for all $g, h \in G$. In fact, they span the space of all class functions on G. Furthermore, they fulfil the relations

$$\chi_{\boldsymbol{R}}(g^{-1}) = \chi_{\boldsymbol{R}}(g)^* = \chi_{\overline{\boldsymbol{R}}}(g)\,, \qquad \forall\, g \in G\,, \tag{4.2a}$$

$$\chi_{\boldsymbol{R}\oplus\boldsymbol{R}'}(g) = \chi_{\boldsymbol{R}}(g) + \chi_{\boldsymbol{R}'}(g)\,, \qquad \forall\, g \in G\,, \tag{4.2b}$$

$$\chi_{\boldsymbol{R}\otimes\boldsymbol{R}'}(g) = \chi_{\boldsymbol{R}}(g) \cdot \chi_{\boldsymbol{R}'}(g)\,, \qquad \forall\, g \in G\,. \tag{4.2c}$$

A character defines uniquely up to equivalence the corresponding representation and vice versa [19].

The representation that belongs to a character $\chi_{\boldsymbol{R}}$ is faithful if and only if $\chi_{\boldsymbol{R}}(g) \neq \dim \boldsymbol{R}$ for all $g \neq e$.

It is possible to define a scalar product on characters. Here, this is shown only for finite groups. Again, the statements stay true for compact groups if the normalised summation is replaced by an integration with respect to the Haar measure.

Definition 22 (Character scalar product [23]). *The scalar product on characters of a group G is defined by*

$$(\chi_{\boldsymbol{R}}, \chi_{\boldsymbol{R}'}) \coloneqq \frac{1}{|G|} \sum_{g\in G} \chi_{\boldsymbol{R}}(g^{-1})\, \chi_{\boldsymbol{R}'}(g) = \frac{1}{|G|} \sum_{g\in G} \chi_{\boldsymbol{R}}(g)^*\, \chi_{\boldsymbol{R}'}(g)\,. \tag{4.3}$$

For irreducible characters this product is one for identical characters and zero for different characters. Hence, the characters of irreducible representations form an orthonormal basis of the space of class functions. This in turn implies that the irreducible characters separate the conjugacy classes, i.e. for any two conjugacy classes there is always a character which takes different values on these classes.

Given a reducible module $\boldsymbol{R}_{\text{red}}$, the multiplicity of the irreducible representation $\boldsymbol{R}_{\text{irr}}$ in $\boldsymbol{R}_{\text{red}}$, i.e. the number of times $\boldsymbol{R}_{\text{irr}}$ is contained in $\boldsymbol{R}_{\text{red}}$, is equal to $(\chi_{\boldsymbol{R}_{\text{irr}}}, \chi_{\boldsymbol{R}_{\text{red}}})$ [23]. In summary, for two representations $\boldsymbol{R}$ on V and $\boldsymbol{R}'$ on W [23],

$$(\chi_{\boldsymbol{R}}, \chi_{\boldsymbol{R}'}) = \dim \operatorname{Hom}_G(V, W)\,. \tag{4.4}$$

The character scalar product can also be used to show that the bijection between representations of a group G and one of its quotient groups G/N is a bijection between irreducible

representations. With the notation of Theorem 5,

$$\begin{aligned}(\chi_{\boldsymbol{R}}, \chi_{\boldsymbol{R}}) = \frac{1}{|G|}\sum_{g\in G}\chi_{\boldsymbol{R}}(g^{-1})\,\chi_{\boldsymbol{R}}(g) &= \frac{|N|}{|G|}\sum_{g\in G/N}\chi_{\boldsymbol{R}}(g^{-1})\,\chi_{\boldsymbol{R}}(g)\\ &= \frac{1}{|G/N|}\sum_{g\in G/N}\chi_{r\circ p}(g^{-1})\,\chi_{r\circ p}(g) = (\chi_{r\circ p}, \chi_{r\circ p})\,.\end{aligned} \tag{4.5}$$

Thus, either both norms are one and both representations are irreducible or both norms are greater than one and neither representation is irreducible.

It also follows directly from (4.3) that the product of two irreducible representations $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$ contains the trivial representation $\boldsymbol{R}_{\mathrm{id}}$ if and only if $\boldsymbol{R}_i = \overline{\boldsymbol{R}}_j$ and then exactly once because

$$(\chi_{\boldsymbol{R}_i\otimes\boldsymbol{R}_j}, \chi_{\boldsymbol{R}_{\mathrm{id}}}) = (\chi_{\boldsymbol{R}_i}\cdot\chi_{\boldsymbol{R}_j}, \chi_{\boldsymbol{R}_{\mathrm{id}}}) = (\chi_{\boldsymbol{R}_i}, \chi_{\overline{\boldsymbol{R}}_j}) = \delta_{\boldsymbol{R}_i,\overline{\boldsymbol{R}}_j}\,. \tag{4.6}$$

II.5 Real and pseudo-real representations

Finite-dimensional representations can be classified according to their relation to their complex conjugate representations. Without loss of generality it is assumed that all representations are unitary.

Definition 23. *A representation $\boldsymbol{R}$ is called*

(i) real if $\boldsymbol{R} \cong \overline{\boldsymbol{R}}$ and if there is a basis such that $\rho_{\boldsymbol{R}}(g)$ is real for all g;

(ii) pseudo-real if $\boldsymbol{R} \cong \overline{\boldsymbol{R}}$ but there is no basis such that $\rho_{\boldsymbol{R}}(g)$ is real for all g;

(iii) complex if $\boldsymbol{R} \ncong \overline{\boldsymbol{R}}$.

Distinguishing between pseudo-real and real representations on the one hand and complex representations on the other hand is simple.

Theorem 11 (Real characters afford (pseudo-) real representations [19])**.** *An irreducible representation is real or pseudo-real if and only if the corresponding character is real for each group element.*

The distinction between real and pseudo-real representations is somewhat more subtle. If a representation $\boldsymbol{R}$ is real or pseudo-real, its representation matrices are related to their complex conjugates by a common similarity transformation,

$$\rho_{\overline{\boldsymbol{R}}}(g) = \rho_{\boldsymbol{R}}(g)^* = U\,\rho_{\boldsymbol{R}}(g)\,U^{-1}\,, \qquad \forall\, g\in G\,, \tag{5.1}$$

with some unitary matrix U. Iterating this equation one finds

$$\rho(g) = (U\,U^*)\,\rho(g)\,(U\,U^*)^{-1}\,, \qquad \forall\, g\in G\,. \tag{5.2}$$

For an irreducible representation $\boldsymbol{R}$, Schur's lemma (Theorem 9) implies that [19]

$$U\,U^* = \pm\mathbb{1}\,. \tag{5.3}$$

Here the plus sign refers to a real representation and the minus sign to a pseudo-real representation, as can be seen as follows.[1]

1 The effect of specific choices of bases for scalar fields in real representations is discussed in Section A.2.

Assume that $U\,U^* = \mathbb{1}$, which implies that U is symmetric,

$$U = U^T\,. \tag{5.4}$$

Hence, one can write

$$U = V\,V^T \tag{5.5}$$

with a unitary matrix V using a Takagi factorisation, see Section A.6.3. After a basis change with V,

$$\rho_{\boldsymbol{R}}(g)' := V^T\,\rho_{\boldsymbol{R}}(g)\,V^*\,, \qquad \forall\, g \in G\,, \tag{5.6}$$

the new matrices $\rho_{\boldsymbol{R}}(g)'$ are manifestly real.

Assuming instead that $U\,U^* = -\mathbb{1}$, U is anti-symmetric, i.e.

$$U = -U^T\,. \tag{5.7}$$

Hence, as can be seen from the normal form of unitary matrices derived in [24] (see also Section A.6.4), it can be written as

$$U = V\,Q\,V^T\,, \tag{5.8}$$

where Q is block-diagonal with blocks of the form

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\,, \tag{5.9}$$

and it is impossible to rotate to a manifestly real basis.

It is possible to distinguish between real, pseudo-real and complex representations using only characters. The means to this is provided by the following theorem.

Theorem 12 (Frobenius–Schur indicator [19])**.** *For a finite group G and a finite-dimensional representation $\boldsymbol{R}$, the Frobenius–Schur indicator is defined by*

$$\mathrm{FS}(\boldsymbol{R}) := \frac{1}{|G|}\sum_{g\in G}\chi_{\boldsymbol{R}}(g^2)\,. \tag{5.10}$$

On irreducible representations $\boldsymbol{R}_i$, it only assumes the values

$$\mathrm{FS}(\boldsymbol{R}_i) = \begin{cases} 1\,, & \text{for } \boldsymbol{R}_i \text{ real,} \\ 0\,, & \text{for } \boldsymbol{R}_i \text{ complex,} \\ -1\,, & \text{for } \boldsymbol{R}_i \text{ pseudo-real.} \end{cases} \tag{5.11}$$

The Frobenius–Schur indicator can also be used for compact groups after replacing the sum with the appropriate integral.

II.6 The tensor product of representations and Clebsch–Gordan coefficients

The concept of the tensor product of representations is crucial for the construction of Lagrangians. Since some of the results presented in this work specifically depend on the tensor product and its connection to the so-called Clebsch–Gordan coefficients of a group, the discussion in this section is kept rather detailed and explicit.

As always, only finite-dimensional representations are discussed, and their representation matrices are all assumed to be chosen unitary. Let $\boldsymbol{R}$ acting on V and $\boldsymbol{R}'$ acting on W be two representations of a group G, and set $n := \dim V$ and $m := \dim W$. Given two bases e_a with $a = 1, \dots, n$ of V and f_b with $b = 1, \dots, m$ of W, the representations $\boldsymbol{R}$ and $\boldsymbol{R}'$ can be viewed as maps from G to $\mathrm{GL}(n, \mathbb{C})$ and $\mathrm{GL}(m, \mathbb{C})$, respectively. Without loss of generality, the bases are assumed to be orthonormal.

The tensor product space $V \otimes W$ can be defined as the span of the ordered pairs of basis vectors from V and W, where the ordered pairs are called the tensor product of the two basis vectors and denoted by $e_a \otimes f_b$ [19],[2]

$$V \otimes W := \left\langle \{ e_a \otimes f_b \mid a = 1, \dots, n;\ b = 1, \dots, m \} \right\rangle . \tag{6.1}$$

The tensor product of general vectors of V and W can be obtained from this construction by bilinear extension and is independent of the original choice of bases. If V and W are inner product spaces, the natural scalar product on the tensor product space is given by

$$\langle v_1 \otimes w_1,\, v_2 \otimes w_2 \rangle_{V \otimes W} = \langle v_1,\, v_2 \rangle_V \cdot \langle w_1,\, w_2 \rangle_W \tag{6.2}$$

such that with respect to the corresponding norm the basis vectors in equation (6.1) are normalised to one. Using this basis, the tensor product representation $\boldsymbol{R} \otimes \boldsymbol{R}'$ acting on $V \otimes W$ can be viewed as a map from G to the matrix group $\mathrm{GL}(n \cdot m, \mathbb{C})$. In this case, the representation matrices of $\boldsymbol{R} \otimes \boldsymbol{R}'$ are given by the Kronecker products of the representation matrices of $\boldsymbol{R}$ and $\boldsymbol{R}'$,

$$\rho_{\boldsymbol{R} \otimes \boldsymbol{R}'}(g) = \rho_{\boldsymbol{R}}(g) \otimes \rho_{\boldsymbol{R}'}(g) , \qquad \forall\, g \in G . \tag{6.3}$$

The resulting tensor product representation $\boldsymbol{R} \otimes \boldsymbol{R}'$ is, in general, not irreducible. Since finite-dimensional representations of compact groups over $\mathbb{C}$ are completely reducible, see Theorem 8, the tensor product space can be decomposed into a direct sum of invariant subspaces U_k, $V \otimes W = \bigoplus_k U_k$. That is, the product of two representations $\boldsymbol{R}$ and $\boldsymbol{R}'$ is equivalent to a direct sum of irreducible representations,

$$\boldsymbol{R} \otimes \boldsymbol{R}' \cong \bigoplus_k \bigoplus_{j=1}^{\mu(k)} \boldsymbol{R}_k , \tag{6.4}$$

where k runs over all inequivalent irreducible representations and $\mu(k)$ is the multiplicity of any given irreducible representation $\boldsymbol{R}_k$ in the product. This multiplicity can be computed by the character scalar product [25]

$$\mu(k) = (\chi_{\boldsymbol{R} \otimes \boldsymbol{R}'},\, \chi_{\boldsymbol{R}_k}) = (\chi_{\boldsymbol{R}} \cdot \chi_{\boldsymbol{R}'},\, \chi_{\boldsymbol{R}_k}) . \tag{6.5}$$

2 For the more general definition of the tensor product using its universal property, cf. e.g. [23].

The block structure of the respective representation matrices can be made visible by a basis transformation $C_{R\otimes R'}$ such that [25]

$$C_{R\otimes R'}^{-1}\,\left(\rho_R(g)\otimes\rho_{R'}(g)\right)\,C_{R\otimes R'}=\bigoplus_k\bigoplus_{j=1}^{\mu(k)}\rho_{R_k}(g)=\bigoplus_k\left(\mathbb{1}_{\mu(k)}\otimes\rho_{R_k}(g)\right)\,,\qquad\forall\,g\in G\,, \tag{6.6}$$

where $C_{R\otimes R'}\in\mathrm{GL}(n\cdot m,\mathbb{C})$ contains the so-called Clebsch–Gordan coefficients of the group G.[3] In other words, $C_{R\otimes R'}$ is the intertwiner realising the equivalence of equation (6.4). In principle, the matrix $C_{R\otimes R'}$ should be viewed as a multi-index object. Its rows are naturally labelled by a pair of indices (a,b) from $\boldsymbol{R}$ and $\boldsymbol{R}'$, respectively, and its columns can be denoted by k running over all irreducible representations, j running over their multiplicity and an index l for the components of $\boldsymbol{R}_k$. Moreover, the two representations whose tensor product is considered should be displayed. One possible notation is therefore (cf. [25])

$$C_{R\otimes R'}=C^{R,R'}_{ab,kjl}=\left(\begin{array}{cc|cc}\boldsymbol{R}&\boldsymbol{R}'&k&j\\a&b&l&\end{array}\right)\,. \tag{6.7}$$

Although having the advantage of showing all dependences of the Clebsch–Gordan matrix explicitly, for its complexity this notation is scarcely used in the following, i.e. the matrix indices of the representation matrices are conventionally suppressed for simplicity.

The Clebsch–Gordan matrices also depend on the explicit matrix realisations of the representations, i.e. on the choice of bases. Given basis transformations

$$\rho_{R_i}(g)'=S_{R_i}\,\rho_{R_i}(g)\,S_{R_i}^{-1}\,,\qquad\forall\,g\in G\,, \tag{6.8}$$

for all irreducible representations $\boldsymbol{R}_i$, the Clebsch–Gordan coefficients for the tensor product of $\boldsymbol{R}_{i_1}$ with $\boldsymbol{R}_{i_2}$ in the new basis are

$$\begin{aligned}C'_{R_{i_1}\otimes R_{i_2}}&=\left(S_{R_{i_1}}\otimes S_{R_{i_2}}\right)\,C_{R_{i_1}\otimes R_{i_2}}\left(\bigoplus_k\bigoplus_{j=1}^{\mu(k)}S_{R_k}^{-1}\right)\\&=\left(S_{R_{i_1}}\otimes S_{R_{i_2}}\right)\,C_{R_{i_1}\otimes R_{i_2}}\left(\bigoplus_k\left(\mathbb{1}_{\mu(k)}\otimes S_{R_k}^{-1}\right)\right)\,.\end{aligned} \tag{6.9}$$

It is important to note that, even after fixing bases for all irreducible representations, the Clebsch–Gordan matrices $C_{R\otimes R'}$ are not unique. One possibility to reduce this arbitrariness is to demand them be unitary, which is always possible and done hereafter. This ensures that the new basis vectors h_{kjl} of the tensor product space, where k again runs over all inequivalent irreducible representations in the product, j over multiple occurrences thereof and l over the indices of $\boldsymbol{R}_k$, given in terms of the old basis by

$$h_{kjl}:=(e_a\otimes f_b)\,C^{R,R'}_{ab,kjl}\,, \tag{6.10}$$

are orthonormal. Even after this choice, there remains, however, still some ambiguity. In fact, one can multiply $C_{R\otimes R'}$ from the right with a unitary matrix,

$$C_{R\otimes R'}\mapsto C_{R\otimes R'}\left(\bigoplus_k\left(W_k\otimes\mathbb{1}_{\dim R_k}\right)\right)\,, \tag{6.11}$$

3 In principle, the order of representations in the direct sum on the right-hand side is arbitrary. Since a re-ordering only amounts to a re-ordering of columns of $C_{R\otimes R'}$, a specific order is assumed to be fixed without any loss of generality. This has already been used in the second equality of (6.6).

where each W_k is a unitary matrix of dimension $\mu(k)$ [25]. This is the most general transformation on (unitary) Clebsch–Gordan matrices as can be seen by applying Schur's lemma to equation (6.6) (up to the aforementioned re-ordering of representations in the direct sum).[4] For representations with multiplicity one in the product the only freedom left is a complex phase, i.e. a $\mathrm{U}(1)$ ambiguity. More generally, for a representation with multiplicity μ, the ambiguity is a $\mathrm{U}(\mu)$ transformation. These ambiguities have lead to some confusion in the model building literature. Hence, Clebsch–Gordan coefficients and their ambiguities are discussed again with regard to their application in the construction of Lagrangians in Section II.7.

So far, Clebsch–Gordan coefficients have only been defined for tensor products of two representations. The definition can, however, easily be extended to multiple factors, e.g. for three factors

$$C^{-1}_{\boldsymbol{R}\otimes\boldsymbol{R}'\otimes\boldsymbol{R}''}\ \left(\rho_{\boldsymbol{R}}(g)\otimes\rho_{\boldsymbol{R}'}(g)\otimes\rho_{\boldsymbol{R}''}(g)\right)\ C_{\boldsymbol{R}\otimes\boldsymbol{R}'\otimes\boldsymbol{R}''}=\bigoplus_k\left(\mathbb{1}_{\mu(k)}\otimes\rho_{\boldsymbol{R}_k}(g)\right)\,,\qquad\forall\,g\in G\,. \tag{6.12}$$

It is clear, of course, that such multiple factor Clebsch–Gordan matrices can be computed given Clebsch–Gordan coefficients for all pairs of irreducible representations. For example, the Clebsch–Gordan matrix $C_{\boldsymbol{R}_{i_1}\otimes\boldsymbol{R}_{i_2}\otimes\boldsymbol{R}_{i_3}}$ for the corresponding triple tensor product can be computed using the Clebsch–Gordan matrices for tensor products of two irreducible representations $C_{\boldsymbol{R}_i\otimes\boldsymbol{R}_j}$. The result is

$$C_{\boldsymbol{R}_{i_1}\otimes\boldsymbol{R}_{i_2}\otimes\boldsymbol{R}_{i_3}}=\left(C_{\boldsymbol{R}_{i_1}\otimes\boldsymbol{R}_{i_2}}\otimes\mathbb{1}_{\dim\boldsymbol{R}_{i_3}}\right)\left(\bigoplus_k\left(\mathbb{1}_{\mu(k)}\otimes C_{\boldsymbol{R}_k\otimes\boldsymbol{R}_{i_3}}\right)\right)\,, \tag{6.13}$$

where k runs over all irreducible representation in the decomposition of the tensor product of $\boldsymbol{R}_{i_1}$ and $\boldsymbol{R}_{i_2}$. This can inductively be generalised to arbitrary numbers of factors in the tensor product.

II.7 Associativity of the tensor product

Finally, let us mention a subtlety that can often be neglected in model building but that can be crucial in some cases, e.g. when CP invariance of a model is discussed. Since the CP properties of models with discrete symmetries are one of the main topics of the present work, see Chapter VII, these details cannot be glossed over here. The point to be raised concerns the associativity of the tensor product and its bearing on the unique specification of a Lagrangian.

The tensor product is associative by the natural isomorphism

$$\begin{aligned}\cong:\quad (V\otimes W)\otimes U &\to V\otimes(W\otimes U)\,,\\ (v\otimes w)\otimes u &\mapsto v\otimes(w\otimes u)\end{aligned} \tag{7.1}$$

4 By Schur's lemma, the matrix multiplying $C_{\boldsymbol{R}\otimes\boldsymbol{R}'}$ from the right can only be block-diagonal with blocks for each k because the $\boldsymbol{R}_k$ are inequivalent irreducible representations which cannot be intertwined; hence, one can consider each subspace with fixed k separately. For any such subspace, the dimension of the space of intertwiners is $\mu(k)$, and, by demanding the Clebsch–Gordan matrix be unitary, the intertwiners have to be unitary. Moreover, inside each individual irreducible representation space, the intertwiner is a phase times the identity leading to the displayed tensor product structure. This phase from the second factor of the tensor product can finally be absorbed via the bilinearity of the tensor product into the first factor.

such that, in principle, the order of computation does not matter. However, this only holds for the whole expression of the tensor product and fails if the computation is performed without explicitly keeping the basis vectors. The reason is that in intermediate steps different phases are implicitly absorbed into the basis vectors depending on the order of computation.[5]

To discuss the relevance of this issue for model building, take as an example first the tensor product of two vectors $v = v_a\, e_a \in V$ and $w = w_b f_b \in W$, which in model building would be fields in irreducible representations of a symmetry group. The tensor product can, as seen in (6.10) above, not only be written in terms of the canonical tensor product basis but also in the basis obtained from this one by the Clebsch–Gordan coefficients,

$$v \otimes w = v_a\, w_b\, (e_a \otimes f_b) \tag{7.2a}$$
$$= C^{-1}_{kjl,ab}\, v_a\, w_b\, (e_m \otimes f_n)\, C_{mn,kjl} = C^{-1}_{kjl,ab}\, v_a\, w_b\, h_{kjl}\,, \tag{7.2b}$$

where the representation dependence of the Clebsch–Gordan coefficients is suppressed. As an example, consider the tensor product of two $\mathbf{2}_0$ doublets v and w of T′ in the basis by Feruglio et al. [26, Appendix A]. Note that the phase convention from this reference, which is also used in the present section, is different from the one shown in Section A.1.2. The result of this contraction is

$$v \otimes w = v_1\, w_1 (e_1 \otimes f_1) + v_1\, w_2 (e_1 \otimes f_2) + v_2\, w_1 (e_2 \otimes f_1) + v_2\, w_2 (e_2 \otimes f_2) \tag{7.3a}$$
$$= \frac{v_2\, w_1 - v_1\, w_2}{\sqrt{2}}\, \frac{e_2 \otimes f_1 - e_1 \otimes f_2}{\sqrt{2}} + \\ + \begin{pmatrix} \frac{1-\mathrm{i}}{2}\, (v_2\, w_1 + v_1\, w_2) \\ \mathrm{i}\, v_1\, w_1 \\ v_2\, w_2 \end{pmatrix}^T \begin{pmatrix} \frac{1+\mathrm{i}}{2}\, (e_1 \otimes f_2 + e_2 \otimes f_1) \\ -\mathrm{i}\, (e_1 \otimes f_1) \\ (e_2 \otimes f_2) \end{pmatrix}. \tag{7.3b}$$

The term in the second line is the singlet in the tensor product and the terms in the last line give the triplet components. It is customary in the literature only to display the coefficients of the basis but not the basis vectors. This can lead to inconsistencies because it is possible to absorb arbitrary phases into the basis vectors even if one demands them to be normalised to one, i.e.

$$v \otimes w = \left(\mathrm{e}^{\mathrm{i}\,\varphi_1}\, \frac{v_2\, w_1 - v_1\, w_2}{\sqrt{2}}\right) \left(\mathrm{e}^{-\mathrm{i}\,\varphi_1}\, \frac{e_2 \otimes f_1 - e_1 \otimes f_2}{\sqrt{2}}\right) + \\ + \begin{pmatrix} \mathrm{e}^{\mathrm{i}\,\varphi_2}\, \frac{1-\mathrm{i}}{2}\, (v_2\, w_1 + v_1\, w_2) \\ \mathrm{e}^{\mathrm{i}\,\varphi_2}\, \mathrm{i}\, v_1\, w_1 \\ \mathrm{e}^{\mathrm{i}\,\varphi_2}\, v_2\, w_2 \end{pmatrix}^T \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\,\varphi_2}\, \frac{1+\mathrm{i}}{2}\, (e_1 \otimes f_2 + e_2 \otimes f_1) \\ -\mathrm{e}^{-\mathrm{i}\,\varphi_2}\, \mathrm{i}\, (e_1 \otimes f_1) \\ \mathrm{e}^{-\mathrm{i}\,\varphi_2}\, (e_2 \otimes f_2) \end{pmatrix} \tag{7.4}$$

is a valid choice for the decomposition into invariant subspaces for any real numbers φ_1 and φ_2. The choice of phases is, of course, precisely the ambiguity of the Clebsch–Gordan coefficients outlined above. This freedom has been used to arrive at the Clebsch–Gordan coefficients for the Feruglio basis shown in Section A.1.2, which have a better CP transformation behaviour, see Chapter VII. This latter advantage notwithstanding, both phase conventions are admissible, and, without any further arguments like the one with respect to CP, one convention cannot be preferred over the other.

Terms of a Lagrangian invariant under a group G are obtained by projecting onto one-dimensional invariant subspaces, i.e. trivial singlets of G. However, without taking into

5 If the Clebsch–Gordan coefficients are not chosen unitary, the results can also differ by a scale factor.

account the basis vectors, there is no control over this process because the projection is implicit in neglecting the basis vectors from the beginning. This can lead to phase ambiguities in the computation of Lagrangian terms from their tensor product expressions even if one uses unitary Clebsch–Gordan coefficients.

As an example, consider the contraction

$$\mathbf{3} \otimes \mathbf{2}_0 \otimes \mathbf{2}_0 \cong \mathbf{1}_0 \oplus \mathbf{1}_1 \oplus \mathbf{1}_2 \oplus \mathbf{3} \oplus \mathbf{3} \oplus \mathbf{3} \tag{7.5}$$

of T′ in the Feruglio basis. The singlet coefficients of the two different ways to perform the computation are related by[6]

$$(\mathbf{3} \otimes \mathbf{2}_0) \otimes \mathbf{2}_0|_{\text{singlet coefficient}} = \mathrm{e}^{\mathrm{i}\,\pi/4} \cdot \mathbf{3} \otimes (\mathbf{2}_0 \otimes \mathbf{2}_0)|_{\text{singlet coefficient}} \tag{7.6a}$$

and the corresponding basis vectors by

$$(\mathbf{3} \otimes \mathbf{2}_0) \otimes \mathbf{2}_0|_{\text{singlet basis vector}} = \mathrm{e}^{-\mathrm{i}\,\pi/4} \cdot \mathbf{3} \otimes (\mathbf{2}_0 \otimes \mathbf{2}_0)|_{\text{singlet basis vector}}\,. \tag{7.6b}$$

In accordance with the fact that the tensor product is associative, the products of coefficient and basis vector coincide. In contrast to that, the coefficients alone exhibit a phase difference of $\pi/4$.

The problem is amplified if there are several trivial singlets in the tensor product as, for example, in

$$\mathbf{3} \otimes \mathbf{2}_0 \otimes \mathbf{3} \otimes \mathbf{2}_0 = \mathbf{1}_0 \oplus \mathbf{1}_0 \oplus \mathbf{1}_0 \oplus \ldots\,. \tag{7.7}$$

Thus, in the tensor product of two triplets and two doublets there are three one-dimensional invariant subspaces, i.e. there is, in fact, a three-dimensional invariant subspace. Since one can project onto each of the three singlets, there are three different possible Lagrangian terms which, in general, can have three distinct couplings. When specifying these couplings, one has to make sure that it is explicit which coupling belongs to which singlet projection. Otherwise, a given set of couplings does not define the model uniquely. In particular, if the basis vectors are omitted from the calculation, different orders of computation lead to different projections onto the three singlet subspaces. The couplings defining the identical theory for different projections are related by a unitary matrix. In the case at hand, for example,

$$\begin{aligned}
&g_1\,((\mathbf{3} \otimes \mathbf{2}_0)_{\mathbf{2}_0} \otimes (\mathbf{3} \otimes \mathbf{2}_0)_{\mathbf{2}_0})_{\mathbf{1}_0} \\
&\qquad + g_2\,((\mathbf{3} \otimes \mathbf{2}_0)_{\mathbf{2}_1} \otimes (\mathbf{3} \otimes \mathbf{2}_0)_{\mathbf{2}_2})_{\mathbf{1}_0} \\
&\qquad + g_3\,((\mathbf{3} \otimes \mathbf{2}_0)_{\mathbf{2}_2} \otimes (\mathbf{3} \otimes \mathbf{2}_0)_{\mathbf{2}_1})_{\mathbf{1}_0} \\
&= g'_1\,(\mathbf{3} \otimes ((\mathbf{2}_0 \otimes \mathbf{3})_{\mathbf{2}_0} \otimes \mathbf{2}_0)_{\mathbf{3}})_{\mathbf{1}_0} \\
&\qquad + g'_2\,(\mathbf{3} \otimes ((\mathbf{2}_0 \otimes \mathbf{3})_{\mathbf{2}_1} \otimes \mathbf{2}_0)_{\mathbf{3}})_{\mathbf{1}_0} \\
&\qquad + g'_3\,(\mathbf{3} \otimes ((\mathbf{2}_0 \otimes \mathbf{3})_{\mathbf{2}_2} \otimes \mathbf{2}_0)_{\mathbf{3}})_{\mathbf{1}_0}\,,
\end{aligned} \tag{7.8}$$

with

$$\begin{pmatrix} g'_1 \\ g'_2 \\ g'_3 \end{pmatrix} = \frac{1+\mathrm{i}}{3\sqrt{2}} \begin{pmatrix} 1 & -2 & 2 \\ -2 & -2 & -1 \\ -2 & 1 & 2 \end{pmatrix} \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix}\,. \tag{7.9}$$

6 Using the phases from the appendix, there is only a mismatch by a sign factor of -1.

It is therefore necessary to specify the order of computation, e.g. via brackets, and for each step the resulting representation as done in equation (7.8) to define a unique theory. However, this is unfortunately often neglected in the literature, cf. [26, 27] for partially problematic examples. The whole discussion becomes especially important when considering the properties of a model under CP transformations, which depend heavily on the choice of phases for couplings. CP transformations in presence of finite groups are discussed in great detail in Chapter VII.

III Flavour and flavour symmetries

Whereas the gauge sector of the Standard Model is very well motivated and understood, even though a simple gauge group might seem even more natural than the reductive SM gauge group G_{SM}, this is not true for the flavour sector, i.e. the non-gauge interactions of the three generations of matter and the Higgs. Gauge interactions are fully specified by the gauge symmetry group, the value of the gauge coupling and maybe a θ_{QCD}-like parameter. For the flavour sector, however, no such strong organising principle is known and masses and mixing angles in the Standard Model have to be set by hand. This amounts, for example, to six masses, three mixing angles and one phase, i.e. to 10 free parameters, in the quark sector alone. There are many more free parameters in the lepton sector, where one faces the additional difficulty that the structure of the neutrino mass terms is not yet known.

The only free parameter of the flavour sector whose value could easily be explained is the Dirac CP phase δ_{CP}, which would vanish if CP were a symmetry of the Standard Model. However, CP is broken, and due to the present lack of theoretical understanding of this effect one can only parametrise the size of the violation by setting δ_{CP} to the experimentally observed value.

An explanation from fundamental principles or just a deeper understanding of the observed structure and the measured values of these parameters is, of course, highly desirable. However, so far no conclusive solution to this flavour puzzle has been found, cf. also [28] for a recent review of these issues and of some of the theoretical efforts towards their solution.

To lay a foundation for the following discussions, in the first part of this chapter, the flavour sector of the Standard Model is reviewed and some notation is introduced. In particular, the CKM and PMNS matrices are defined, and the phase ambiguities in these definitions are highlighted.

One possible avenue towards a solution to the flavour puzzle is provided by flavour symmetries. Relating different terms of the flavour sector, they at least decrease the number of free parameters. Furthermore, they might provide a reason for the peculiar structures in the quark and lepton sector. The concept of such symmetries is introduced in Section III.2. Of course, given the topic of this text, the focus is set on discrete non-abelian symmetries.

In order to illustrate the use of such discrete non-abelian flavour symmetries, a model for the neutrino sector originally devised by Altarelli and Feruglio [9, 10] is reviewed in Section III.3. This model is based on the symmetry group of a regular tetrahedron A_4. It also serves as an example in later chapters.

Although discrete flavour symmetries are a very promising option, there is some valid criticism of the way they are used in model building. Thus, in the final section of this chapter,

(Left-handed) particles	Symbol ($i = 1, 2, 3$)	$(\mathrm{SU}(3)_\mathrm{C}, \mathrm{SU}(2)_\mathrm{L}, \mathrm{U}(1)_\mathrm{Y})$
lepton doublets	$l_i \coloneqq (\nu_i,\, e_i)^T$	$(\mathbf{1}, \mathbf{2}, -1/2)$
lepton singlets	e_i^c	$(\mathbf{1}, \mathbf{1}, 1)$
singlet neutrinos	ν_i^c	$(\mathbf{1}, \mathbf{1}, 0)$
quark doublets	$q_i \coloneqq (u_i,\, d_i)^T$	$(\mathbf{3}, \mathbf{2}, 1/6)$
up quark singlets	u_i^c	$(\overline{\mathbf{3}}, \mathbf{1}, -2/3)$
down quark singlets	d_i^c	$(\overline{\mathbf{3}}, \mathbf{1}, 1/3)$
Higgs boson	$h \coloneqq (h^+,\, h^0)^T$	$(\mathbf{1}, \mathbf{2}, 1/2)$

Table III.1: Representations and field symbols for all SM matter particles plus right-handed neutrinos written as left-handed Weyl spinors and the Higgs boson [29].

this criticism is briefly discussed and some general comments on the predictiveness of such models are made, concluding the introduction to the flavour problem and to discrete flavour symmetries.

III.1 The flavour sector of the Standard Model

The three generations of matter observed so far in both quark and lepton sector are distinguished not by their gauge interactions but only by their masses, which are determined by their couplings to the Higgs boson, the so-called Yukawa couplings. For the charged lepton and quark sector, they can be written using left-handed Weyl spinors as

$$\begin{aligned}\mathcal{L}_\mathrm{SM} \supset & -Y_e^{ij}\, h^*\, e_i^c\, l_j - Y_d^{ij}\, h^*\, d_i^c\, q_j - Y_u^{ij}\, \epsilon\, h\, u_i^c\, q_j + \mathrm{h.\,c.} \\ & \xrightarrow{\text{EWSB}} -\frac{v}{\sqrt{2}}\, Y_e^{ij}\, e_i^c\, e_j - \frac{v}{\sqrt{2}}\, Y_d^{ij}\, d_i^c\, d_j - \frac{v}{\sqrt{2}}\, Y_u^{ij}\, u_i^c\, u_j + \mathrm{h.\,c.}\end{aligned} \tag{1.1}$$

with the notation for the Standard Model fields summarised in Table III.1 and $v \coloneqq \langle h^0 \rangle$. The Yukawa matrices $Y_{e/u/d}$ are, in the SM, not restricted by any symmetry but arbitrary complex matrices in flavour space. One might therefore expect their entries to be order one complex numbers. Experimentally, however, this turns out not to be the case. It is more convenient to discuss this in the mass basis instead of the flavour basis used in equation (1.1).

The transformation matrices for this change of basis can be obtained from the singular value decomposition, see also Section A.6.2, of the Yukawa matrices,

$$\frac{v}{\sqrt{2}}\, Y_f =: V_f M_f U_f^\dagger\,, \qquad f = e,\, u,\, d\,, \tag{1.2}$$

where M_f is diagonal with real non-negative eigenvalues. The new fields obtained by

$$f_i' \coloneqq (U_f^\dagger)_{ij}\, f_j \tag{1.3a}$$

$$(f^c)_i' \coloneqq f_j^c\, (V_f)_{ji} \tag{1.3b}$$

for $f = e,\, u,\, d$ are the desired mass eigenstates.

Without further assumptions one might expect the masses to be of the order of the Higgs vacuum expectation value (VEV) $v \approx 246\,\mathrm{GeV}$. However, they turn out to be strongly hierarchical with only the top quark mass being of the expected order; all other masses are smaller by one or several orders of magnitude. A possible explanation for this pattern is the Froggatt–Nielsen mechanism [30], which is briefly reviewed in Section III.2.

Since the rotations of left-handed up quarks U_u and down quarks U_d need not be identical, and, in fact, are not so in Nature, the $\mathrm{SU}(2)_\mathrm{L}$ charged current interactions are non-diagonal in the mass eigenstate basis. This mismatch is encoded by the CKM matrix

$$U_\mathrm{CKM} \coloneqq U_u^\dagger\, U_d \tag{1.4}$$

named after Cabibbo [31] and Kobayashi and Maskawa [32]. As a unitary 3×3 matrix, it has 9 free parameters, which can be written as three angles and six phases.[1] However, not all of them are uniquely defined, and, therefore, some are not observable. Indeed, assuming non-degenerate masses, the matrices U_f and V_f are only defined up to multiplication with a diagonal phase matrix ,

$$V_f \mapsto V_f\, U_f^\mathrm{ph}\,, \tag{1.5a}$$

$$U_f \mapsto U_f\, U_f^\mathrm{ph}\,, \tag{1.5b}$$

see also Section A.6.2, which represents nothing but the freedom to re-phase the quark fields. Hence, the CKM matrix is only defined up to the transformation

$$U_\mathrm{CKM} \mapsto (U_u^\mathrm{ph})^\dagger\, U_\mathrm{CKM}\, U_d^\mathrm{ph}\,, \tag{1.6}$$

which can be used to remove five out of the six phases (U_CKM is invariant under changes of the overall common phase of $U_{u/d}^\mathrm{ph}$). The CKM matrix is conventionally written as the product [33]

$$U_\mathrm{CKM} = \mathrm{diag}\,(\mathrm{e}^{\mathrm{i}\,\delta_u},\, \mathrm{e}^{\mathrm{i}\,\delta_c},\, \mathrm{e}^{\mathrm{i}\,\delta_t})\; V(\theta_{12}, \theta_{13}\,\theta_{23}, \delta_{CP})\; \mathrm{diag}\,(\mathrm{e}^{-\mathrm{i}\,\alpha_1/2},\, \mathrm{e}^{-\mathrm{i}\,\alpha_2/2},\, 1) \tag{1.7}$$

with

$$V = \begin{pmatrix} c_{12}\,c_{13} & s_{12}\,c_{13} & s_{13}\,\mathrm{e}^{-\mathrm{i}\,\delta_{CP}} \\ -s_{12}\,c_{23} - c_{12}\,s_{23}\,s_{13}\,\mathrm{e}^{\mathrm{i}\,\delta_{CP}} & c_{12}\,c_{23} - s_{12}\,s_{23}\,s_{13}\,\mathrm{e}^{\mathrm{i}\,\delta_{CP}} & s_{23}\,c_{13} \\ s_{12}\,s_{23} - c_{12}\,c_{23}\,s_{13}\,\mathrm{e}^{\mathrm{i}\,\delta_{CP}} & -c_{12}\,s_{23} - s_{12}\,c_{23}\,s_{13}\,\mathrm{e}^{\mathrm{i}\,\delta_{CP}} & c_{23}\,c_{13} \end{pmatrix}, \tag{1.8}$$

using $s_{ij} \coloneqq \sin\theta_{ij}$ and $c_{ij} \coloneqq \cos\theta_{ij}$. In this parametrisation $\theta_{ij} \in [0,\, \pi/2]$ and $\delta_f,\, \delta_{CP},\, \alpha_i \in [0,\, 2\,\pi]$. The physical parameters are the angles θ_{ij} and the CP violating (Dirac) phase δ_{CP}. The other phases are removable by the transformation shown above.[2]

Among these parameters, the Dirac phase δ_{CP} is special because it is so far the only experimentally verified source of CP violation in the Standard Model. If it were trivial, i.e. zero or π, CP could still be a symmetry of the SM.[3] CP symmetries and their violation are discussed in detail in Chapter VII.

1 In general, a $n \times n$ unitary matrix has $2\,n^2 - n^2 = n^2$ parameters of which $1/2\,n\,(n-1)$ are angles which span the subspace of orthogonal matrices.

2 Note that this transformation is, in general, chiral and therefore affects the vacuum angle of QCD.

3 Of course, CP has to be violated for baryogenesis [34].

$\sin\theta_{12}$	$\sin\theta_{23}$	$\sin\theta_{13}$	$\delta_{CP}/^\circ$
0.22523 ± 0.00065	0.0417 ± 0.00057	0.00363 ± 0.00012	69.4 ± 3.4

Table III.2: Pre-ICHEP2014 values for mixing angles and phases of the CKM matrix by the UTfit collaboration [35].

Instead of the anarchic structure that might be expected due to the absence of any organising principle for the Yukawa couplings, the observed magnitudes of the U_{CKM} matrix are highly diagonal [33]:

$$|U_{\mathrm{CKM}}| \approx \begin{pmatrix} 0.974 & 0.225 & 0.004 \\ 0.225 & 0.973 & 0.041 \\ 0.009 & 0.041 & 0.999 \end{pmatrix} . \tag{1.9}$$

Values for the angles and δ_{CP} can be found in Table III.2. It is tempting to assume that this structure of U_{CKM} is the perturbation of a unit matrix, e.g. via quantum effects or a softly broken symmetry. However, it is also possible to arrive at a CKM matrix consistent with observation by the use of discrete non-abelian flavour symmetries, cf. e.g. [36]. An explanation of the general structure of such models, albeit with a focus on the lepton sector, is deferred to Section III.2.

The discussion can be repeated for the neutrino sector with the additional difficulty that it is not yet known how neutrinos obtain their masses. So far, it has not even been possible to determine whether the observed three light neutrinos are Dirac or Majorana particles, i.e. whether lepton number is conserved. The different possibilities how mass terms can be generated are not presented here in detail, cf. [37, 38] and references therein for more information. Moreover, the discussion is focused on the case of the three light active SM neutrinos with the possible addition of three total singlet neutrinos.[4] This is in complete agreement with the number of light neutrinos determined from, for example, the Z^0 width [33] and also with the number required for anomaly freedom of the SM. For the more general case of arbitrary neutrino numbers, cf. [39].

The notion of Dirac neutrinos means that there is a pure (effective) Dirac mass term coupling the left-handed neutrinos from the lepton doublets of the SM to additional singlet neutrinos ν_i^c. Such a term is, of course, not $\mathrm{SU}(2)_{\mathrm{L}}$ gauge invariant but can be generated by one insertion of the SM Higgs. After plugging in the vacuum expectation value of the Higgs, one obtains a mass term of the form

$$\mathcal{L}_{m_\nu} = -m_D^{ij}\, \nu_i^c\, \nu_j + \mathrm{h.\,c.} \tag{1.10}$$

This term is, for the natural assignment of charges, invariant under lepton number transformations.

The mass eigenstates can be determined in complete analogy to the quark case. Although the absolute neutrino mass scale has not been measured directly, there are upper bounds on it. The presently strongest upper bound on the total mass of active neutrinos is derived from cosmological considerations and observations [40],

$$\sum_i m_{\nu_i} < 0.23\,\mathrm{eV}\,. \tag{1.11}$$

4 Usually, these neutrinos are referred to as 'right-handed' neutrinos. However, in the present notation they are, like all other matter fields, written as left-handed Weyl spinors. Therefore, they are most often called singlet neutrinos hereafter.

Thus, neutrino masses are of the order 0.1 eV comparing to the 0.511 MeV of the electron. Since the Dirac mass terms for charged leptons and neutrinos are structurally identical, it seems difficult, albeit not impossible (cf. e.g. [41]), to explain this huge hierarchy between the mass scales in a natural fashion. This is easier for the Majorana case where the See-saw mechanism can be employed, see below.

The discussion of the mixing matrix, which in the lepton sector is called PMNS matrix after Pontecorvo [42] and Maki, Nakagawa and Sakata [43], proceeds precisely as in the quark case defining[5]

$$U_{\text{PMNS}} := U_e^\dagger \, U_\nu \,. \tag{1.12}$$

In contrast to Dirac neutrinos, Majorana neutrinos, which are their own anti-particles, allow for a Majorana mass term. Given only the SM field content, this can arise via the effective Weinberg operator [44] at the non-renormalisable level,

$$\begin{aligned} \mathcal{L}_{m_\nu} &= \frac{1}{4} \, \kappa^{ij} \, (\nu_i \, \varepsilon \, h) \, (\nu_j \, \varepsilon \, h) + \text{h. c.} \\ &\xrightarrow{\text{EWSB}} \frac{1}{2} \, m_\nu^{ij} \, \nu_i \, \nu_j + \text{h. c.} \end{aligned} \tag{1.13}$$

with $m_\nu = v^2 \, \kappa / 4$ and where the couplings κ^{ij} have negative mass dimension. Using the Weinberg operator one is agnostic about the specific type of interaction that, at the fundamental level, generates the neutrino masses. However, it assumes that the relevant degrees of freedom are heavy compared to the energies involved in the observed processes.

There is a popular natural solution to generate a Majorana mass term with the desired suppression with respect to the charged lepton masses: the (type I) See-saw mechanism [45–48]. Here both Dirac and Majorana mass terms exist,

$$\mathcal{L}_{m_\nu} = -m_D^{ij} \, \nu_i^c \, \nu_j - m_R^{ij} \, \nu_i^c \, \nu_j^c + \text{h. c.} \,, \tag{1.14}$$

but the Majorana masses are much larger than the Dirac masses. Then the combined mass matrix for ν_i and ν_i^c can be approximately block-diagonalised yielding

$$\mathcal{L}_{m_\nu} \approx m_\nu^{ij} \, \nu_i' \, \nu_j' - m_R^{ij} \, (\nu^c)_i' \, (\nu^c)_j' + \text{h. c.} \,, \tag{1.15}$$

with $m_\nu \approx -m_D^T \, m_R^{-1} \, m_D$, $\nu_i' \approx \nu_i$ and $(\nu^c)_i' \approx \nu_i^c$ for large m_R [49]. Hence, the masses for ν_i are suppressed by the Majorana mass of the ν_i^c, which is the origin of the name See-saw. Putting the Majorana masses at the GUT scale of 10^{16} GeV and the Dirac masses at the electroweak scale v yields neutrinos too light by one to two orders of magnitude. This can be ameliorated, for example, by using a lower scale for the right-handed neutrinos or by a large number of right-handed neutrinos as in certain string models [50].

Since Majorana mass terms have a different structure than Dirac mass terms, one cannot use a simple singular value decomposition to compute the mass eigenstates. However, the Majorana mass matrix is symmetric, and it can be diagonalised by a Takagi factorisation, see also Section A.6.3,

$$m_\nu = U_\nu^* \, D_\nu \, U_\nu^\dagger \,, \tag{1.16}$$

5 This is the adjoint of the CKM matrix definition when written in terms of $\text{SU}(2)_\text{L}$ doublet components.

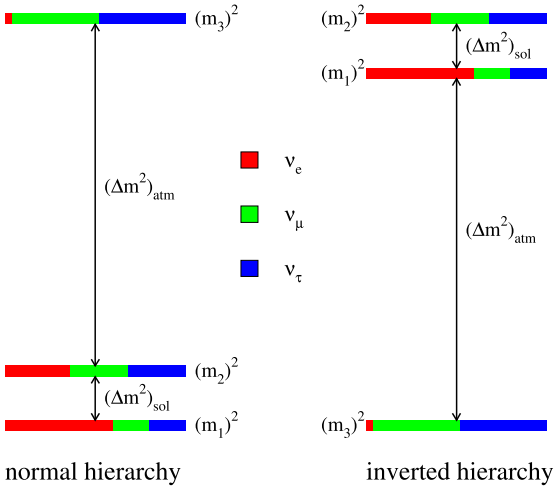

Figure III.1: The two possible neutrino mass hierarchies are depicted. The colours denote the fraction of each flavour state $\nu_{e,\mu,\tau}$ contained in the mass eigenstates $\nu_{1,2,3}$, i.e. the boxes are partitioned according to the absolute values squared of the corresponding entries in U_{PMNS}. This figure is taken from [53].

where D_ν is diagonal with real non-negative eigenvalues. Hence, the unitary matrix U_ν is not defined up to multiplication with a diagonal phase matrix like in the quark sector but up to

$$U_\nu \mapsto U_\nu \text{ diag}\,(\pm 1, \pm 1, \pm 1)\,. \tag{1.17}$$

Thus, the phases α_i, called Majorana phases, in the PMNS analogue to (1.7) cannot be removed by a re-phasing of the neutrino fields and are, hence, physical. Aside from this, the mixing matrix U_{PMNS} can be computed as for Dirac neutrinos.

In both Dirac and Majorana cases, the misalignment of flavour and mass eigenstates leads to the well-known phenomenon of neutrino oscillations [42]. Oscillation amplitudes only depend on the mixing angles θ_{ij}, δ_{CP} and the differences Δm^2_{ij} of the squared masses of neutrinos but not on the Majorana phases or the absolute mass scale. In contrast to the quark sector, not all lepton masses and mixing parameters have been measured. The absolute values of the differences of the squared masses are known and also that $\Delta m^2_{21} > 0$ from the MSW effect [51, 52], whereas the absolute mass scale as well as the sign of Δm^2_{31} are unknown. Thus, ν_3 could be the heaviest (normal ordering) or lightest (inverted ordering) state, see Figure III.1. Moreover, all three mixing angles have been measured, but the Dirac CP phase δ_{CP} and the Majorana phases are still unknown.[6]

The absolute values of the entries of the PMNS matrix do not show the same almost diagonal structure as the CKM entries without, however, being totally devoid of any structure [54]:

$$|U_{\text{PMNS}}|_{3\sigma} = \begin{pmatrix} 0.801 \to 0.845 & 0.514 \to 0.580 & 0.137 \to 0.158 \\ 0.225 \to 0.517 & 0.441 \to 0.699 & 0.614 \to 0.793 \\ 0.246 \to 0.529 & 0.464 \to 0.713 & 0.590 \to 0.776 \end{pmatrix} \tag{1.18}$$

6 Majorana phases are only physical and therefore measurable if the neutrinos are Majorana neutrinos, of course.

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	Normal Ordering ($\Delta\chi^2 = 0.97$)		Inverted Ordering (best fit)		Any Ordering
	bfp $\pm 1\sigma$	3σ range	bfp $\pm 1\sigma$	3σ range	3σ range
$\sin^2\theta_{12}$	$0.304^{+0.013}_{-0.012}$	$0.270 \to 0.344$	$0.304^{+0.013}_{-0.012}$	$0.270 \to 0.344$	$0.270 \to 0.344$
$\theta_{12}/^\circ$	$33.48^{+0.78}_{-0.75}$	$31.29 \to 35.91$	$33.48^{+0.78}_{-0.75}$	$31.29 \to 35.91$	$31.29 \to 35.91$
$\sin^2\theta_{23}$	$0.452^{+0.052}_{-0.028}$	$0.382 \to 0.643$	$0.579^{+0.025}_{-0.037}$	$0.389 \to 0.644$	$0.385 \to 0.644$
$\theta_{23}/^\circ$	$42.3^{+3.0}_{-1.6}$	$38.2 \to 53.3$	$49.5^{+1.5}_{-2.2}$	$38.6 \to 53.3$	$38.3 \to 53.3$
$\sin^2\theta_{13}$	$0.0218^{+0.0010}_{-0.0010}$	$0.0186 \to 0.0250$	$0.0219^{+0.0011}_{-0.0010}$	$0.0188 \to 0.0251$	$0.0188 \to 0.0251$
$\theta_{13}/^\circ$	$8.50^{+0.20}_{-0.21}$	$7.85 \to 9.10$	$8.51^{+0.20}_{-0.21}$	$7.87 \to 9.11$	$7.87 \to 9.11$
$\delta_{\rm CP}/^\circ$	306^{+39}_{-70}	$0 \to 360$	254^{+63}_{-62}	$0 \to 360$	$0 \to 360$
$\frac{\Delta m^2_{21}}{10^{-5}\ \text{eV}^2}$	$7.50^{+0.19}_{-0.17}$	$7.02 \to 8.09$	$7.50^{+0.19}_{-0.17}$	$7.02 \to 8.09$	$7.02 \to 8.09$
$\frac{\Delta m^2_{3\ell}}{10^{-3}\ \text{eV}^2}$	$+2.457^{+0.047}_{-0.047}$	$+2.317 \to +2.607$	$-2.449^{+0.048}_{-0.047}$	$-2.590 \to -2.307$	$\begin{bmatrix}+2.325 \to +2.599\\ -2.590 \to -2.307\end{bmatrix}$

Table III.3: Table from [54] showing the values for the neutrino mixing parameters and mass splittings from their global fit.

The results of a global fit to neutrino data for the mass splittings and mixing angles are shown in Table III.3. On the one hand, the structure that emerges in the PMNS matrix could be described as the perturbation of one of several symmetric mixing matrices, where the latter can be obtained at first order from discrete non-abelian flavour symmetries, see the subsequent section. On the other hand, the mixing matrix is still consistent with the assumption of anarchy [55, 56], i.e. precisely the absence of any organising principle, an avenue that is not pursued further in this work.

III.2 Flavour symmetries

As seen in the previous section, the flavour structure of the Standard Model clearly asks for an explanation, i.e. for a derivation from fundamental principles. However, there has not yet emerged any definite strategy to reach this goal. One important candidate is the idea of flavour symmetries, cf. [28, 37, 38, 57–59] for reviews. In this approach, it is assumed that there is a fundamental symmetry acting on flavour space and supplying relations between different Yukawa couplings. In order to generate non-degenerate masses for the SM particles, this symmetry must be broken somewhere above the electroweak scale. It may then be hoped that the relations between couplings enforced by the additional symmetry constrain the possible flavour patterns even after the breaking, providing an explanation for the observed structure. In the best case, this also explains the observed CP violation in the SM.

It is clear that, before building a concrete model, one has to make some fundamental decisions about the preferred type of symmetry and the method of breaking. Firstly, the symmetry can be abelian or non-abelian, discrete or continuous and gauged or global. Secondly, the breaking can be explicit or spontaneous or by certain geometric means of higher-dimensional models. Every choice has specific advantages and disadvantages.

As method of breaking, spontaneous symmetry breaking is generally to be preferred over

explicit breaking. For an explicitly broken symmetry one should have reasons why the symmetry should hold approximately instead of being wholly absent. Moreover, the size of the breaking is usually very important for the phenomenology of approximate symmetries, controlling how 'approximate' the symmetry is and therefore how predictive it is despite being broken. This can, without any further arguments, induce a fine-tuning for the couplings of the symmetry breaking operators. An exception are approximate symmetries which arise if an exact discrete symmetry is accidentally enlarged to an approximate continuous symmetry that is only broken by higher-order operators, cf. e.g. [60]. In this case, the effective field theory suppression can yield the desired explanation for the smallness of the explicit breaking.

Regarding the type of symmetry used, note that global continuous symmetries have two important disadvantages. The first issue is that global symmetries are believed to be broken by gravitational effects [12, 13]. Secondly, if global continuous symmetries are spontaneously broken, one has to deal with the emerging Goldstone bosons, which severely challenge the phenomenological viability of such models. Both issues could be disposed of by gauging the symmetry: gauge symmetries are safe from violations by quantum gravity [61] and Goldstone modes are absorbed by the gauge bosons.

The alternative are discrete flavour symmetries, which do not suffer from any problems associated to Goldstone bosons and for which also solutions exist that overcome the first issue. One possible consistent origin of these symmetries that shields them from gravitational violation is, for example, provided by string theory [62]. Another possibility is starting with a gauged continuous symmetry at very high energies, which is then broken spontaneously to the discrete symmetry; an avenue that is investigated more thoroughly in Chapter VI.

The focus of this work is on discrete symmetries; however, it is instructive to discuss the simplest type of flavour symmetry first, which is a (gauged) abelian $\mathrm{U}(1)$ symmetry.[7] This leads to models of the Froggatt–Nielsen type [30], which can be used to explain the mass hierarchy among generations. The fundamental observation is that Yukawa terms like

$$\mathcal{L}_m \supset -Y^e\, h^*\, e^c\, e \tag{2.1}$$

are forbidden if the charges q_f of matter fields under the Froggatt–Nielsen $\mathrm{U}(1)_{\mathrm{FN}}$ are non-negative integers that depend on the generation while no other SM field carries a charge. The reason is that, by assumption, $q_{e^c} + q_e > 0$ and analogously for the other matter fields besides maybe the top quark, for which an order one Yukawa coupling is desirable. Introducing an additional scalar field φ, called flavon, uncharged with respect to $\mathrm{G_{SM}}$ but with negative charge $q_\varphi = -1$ with respect to $\mathrm{U}(1)_{\mathrm{FN}}$, the higher-order terms

$$\mathcal{L}_m \supset -\left(\frac{\varphi}{\Lambda}\right)^{q_{e^c}+q_e} Y^e\, h^*\, e^c\, e \tag{2.2}$$

are invariant under all symmetries. The mass scale Λ is, as usual, assumed to be some high scale associated with new physics, which can be the Planck or some lower scale, depending on the model. If the flavon VEV $\langle\varphi\rangle$ is smaller than the new physics scale, e.g. of the order of $0.1\,\Lambda$, the mass terms are suppressed by powers of a small quantity. Depending on the precise value of the flavon VEV one adjusts the $\mathrm{U}(1)_{\mathrm{FN}}$ charges such that a viable mass hierarchy emerges from this process. For a discussion of the Froggatt–Nielsen mechanism in a supersymmetric context and of its relation to GUTs and anomaly cancellation by the Green–Schwarz mechanism [64], cf. [65–68]. Similarly suppressed Yukawa couplings can

7 It is also possible to build very similar models with $\mathbb{Z}_N$ symmetries, cf. e.g. [63].

be obtained without a Froggatt–Nielsen symmetry by coupling the model to a strongly coupled sector which generates the suppression due to the running of the wave function renormalisation factors [69, 70].

Since by Theorem 3 abelian groups only have one-dimensional irreducible representations, it is clear that they cannot yield any non-trivial predictions for the mixing of quarks or leptons. It is just impossible to obtain relations between different generations, i.e. between two or more fields, using one-dimensional representations. Only non-abelian groups feature the higher-dimensional irreducible representations that are needed for these relations. Non-abelian groups also have the advantage that they can suppress the additional contributions to flavour changing neutral currents (FCNCs) that many models of physics beyond the Standard Model introduce. Stringent experimental bounds, which challenge models of new physics, exist for many of these processes, e.g. for the lepton sector $\mathrm{Br}(\mu^+ \to e^+ + \gamma) < 5.7 \cdot 10^{-13}$ [71]. Non-abelian flavour symmetries ameliorate the problem by restricting the number of inter-generational operators allowed. This is, in particular, also true for certain discrete symmetries, cf. [72].

Summarising their benefits, discrete non-abelian flavour symmetries can be shielded from gravitational violations, they do not suffer from the prediction of unobserved Goldstone bosons, they can be used to generate non-trivial mixing structures and they suppress FCNCs. Therefore, they can be considered favourable tools for model building. Information on many groups used in model building can be found in [57, 58, 73, 74]. Details for some of them are also compiled in Section A.1.

As the focus of this text is on such discrete non-abelian groups, it seems advisable to be a bit more precise regarding the terminology 'discrete'. Discrete groups are, from now on, understood to be subgroups of $\mathrm{GL}(n, \mathbb{C})$ for some $n \in \mathbb{N}$ that, with respect to the subgroup topology, are discrete. In fact, the notion shall be even further restricted in the non-abelian case to compact groups, which are then automatically finite. Simply speaking this implies that 'discrete group' refers to either a finite abelian or non-abelian group or such a group with additional factors of $\mathbb{Z}$.

As an aside, note that, especially in neutrino model building, there is sometimes made a distinction between so-called 'direct' and 'indirect' models [37, 75]. This terminology is related to the automatic symmetries of Dirac and Majorana mass matrices. A Majorana mass matrix is invariant under $\mathbb{Z}_2^3$ transformations acting on the lepton doublets, and a Dirac mass matrix is invariant under $\mathrm{U}(1)^3$ (cf. e.g. [76]). This is also reflected in the freedom to remove signs and phases from the mixing matrices, see (1.5) and (1.17). Usually, overall phase transformations are divided out of these symmetries; hence, one speaks of the Klein symmetry $\mathbb{Z}_2 \times \mathbb{Z}_2$ of the Majorana mass matrix and of $\mathrm{U}(1) \times \mathrm{U}(1)$ as symmetry of the Dirac masses. Models in which the Klein symmetry and a finite (usually $\mathbb{Z}_3$) subgroup of $\mathrm{U}(1)^2$ are contained in the original flavour symmetry are called direct models. In this case the flavour symmetry is broken to two different subgroups in the neutrino and charged lepton sector containing the respective mass matrix symmetries. If a direct model is to yield tri-bi-maximal mixing, the flavour group must contain the permutation group on four letters S_4 [77, 78]. In the indirect approach, the symmetries of the mass matrices are not contained in the original flavour symmetry group and arise accidentally, putting the focus on the exact alignment of the flavon vacuum expectation values. For a pictorial comparison of these differences of the direct and indirect model building approaches, see also Figure III.2.

As already mentioned above, the PMNS matrix does not seem to be the perturbation of a unit matrix, in contrast to the CKM matrix. However, there are certain popular propositions for mixing matrices that arise at first order in flavour models and that could be the correct

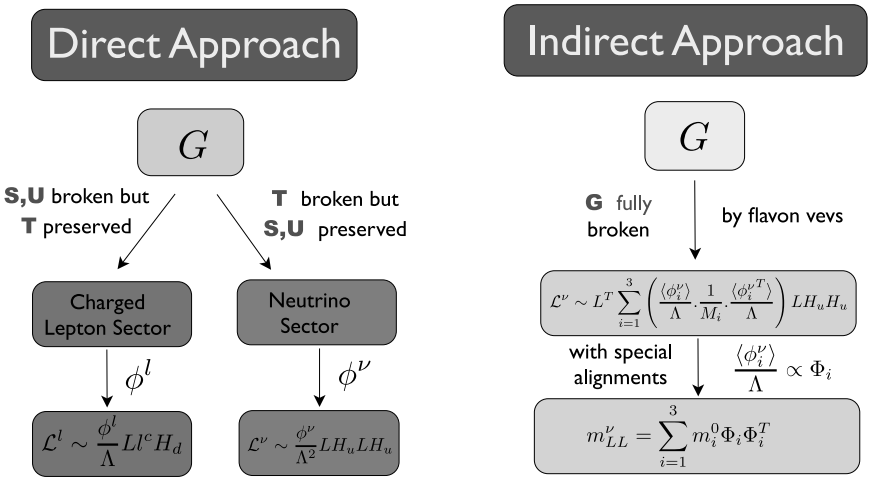


Figure III.2: Comparison of the direct and indirect model building approaches, figure taken from [79].

	bi-maximal	tri-bi-maximal	golden ratio
$\tan\theta_{12}$	1	$1/\sqrt{2}$	$2/(1+\sqrt{5})$
$\theta_{12}/^\circ$	45	35.26	31.72

Table III.4: Values of the mixing angle θ_{12} for bi-maximal, tri-bi-maximal and golden ratio mixing [37].

starting point for an explanation of the structure of U_{PMNS}. The three particularly popular shapes of bi-maximal [80, 81], tri-bi-maximal [82] and golden ratio mixing [83, 84] share the properties $\theta_{13} = 0^\circ$ and $\theta_{23} = 45^\circ$ such that [37]

$$U_{\text{PMNS}} = \begin{pmatrix} c_{12} & s_{12} & 0 \\ -\frac{s_{12}}{\sqrt{2}} & \frac{c_{12}}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{s_{12}}{\sqrt{2}} & -\frac{c_{12}}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}, \tag{2.3}$$

where both Majorana and charged lepton phases are set to zero. The remaining angle θ_{12} for all three cases is shown in Table III.4. Of the three cases, the tri-bi-maximal mixing matrix

$$U_{\text{TBM}} := \begin{pmatrix} \sqrt{\frac{2}{3}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{pmatrix} \tag{2.4}$$

plays the most important role in the following. All three propositions share the deficiency that θ_{13} is predicted to be exactly zero. This is a remnant of the times before the direct measurement of this angle [85–89] when the observational results were still consistent with zero. Note that $\theta_{13} = 0$ implies that the CP phase δ_{CP} is not well defined.

Before providing an example for models with discrete non-abelian flavour symmetries leading to such mixing matrices in the next section, two more general remarks are in order.

First, note that it can be shown that the symmetry group has to be fully broken, i.e. broken to at most an abelian subgroup, to arrive at a realistic pattern of masses and mixing

	l	e^c	μ^c	τ^c	h_u	h_d	φ_e	φ_ν	ξ
A_4	**3**	**1**	**1″**	**1′**	**1**	**1**	**3**	**3**	**1**
$\mathbb{Z}_4$	1	3	3	3	0	0	0	2	2
$\langle\cdot\rangle$	0	0	0	0	$\begin{pmatrix}0\\v_u\end{pmatrix}$	$\begin{pmatrix}v_d\\0\end{pmatrix}$	$\begin{pmatrix}v'\\0\\0\end{pmatrix}$	$\begin{pmatrix}v\\v\\v\end{pmatrix}$	w

Table III.5: The A_4 representations and $\mathbb{Z}_4$ charges of all fields relevant to the lepton sector of the model by Altarelli and Feruglio [9, 10]. Additionally, the vacuum expectation values after flavour and electroweak symmetry breaking are displayed.

parameters [90]. The reason is that, if some non-abelian subgroup stayed unbroken, there would be degenerate masses or some mixing angles would vanish contradicting experimental observations.

The second point concerns the spontaneous breaking of any discrete symmetry. In principle, the physical vacua in causally disconnected patches of the universe can be equivalent but different. Such vacua are connected by the symmetry transformations that are spontaneously broken. For discrete symmetries, regions living in different vacua are thus separated by domain walls [91] as there is no way continuously to deform one vacuum solution into a different but equivalent one. No such domain wall has been observed; hence, for a model to be viable one must either hide or annihilate them. Possible solutions are the use of (pseudo-) anomalous symmetries for which the domain walls can dissolve due to the anomalous breaking of the symmetry [92] or, again, discrete gauge symmetries for which the different vacua are not equivalent but actually identical. Using the former solution there is, of course, the difficulty that the anomaly might change the phenomenology of a model in many more ways than just the annihilation of domain walls. Anomalies of discrete groups are considered in detail in Chapter IV.

III.3 Example model with A_4 symmetry

It is most instructive to discuss flavour models with discrete non-abelian symmetries by means of a specific example. The chosen one is a model by Altarelli and Feruglio [9, 10]. It is based on the alternating group on four letters A_4, which is also called tetrahedral group since it is the symmetry group of a regular tetrahedron. For details of A_4, see Section A.1.1.[8] The model predicts tri-bi-maximal mixing for the neutrinos at first order. Regarding the terminology introduced before, since clearly A_4 does not contain S_4, the model is not a fully direct model. However, it is sometimes called a semi-direct model as only one $\mathbb{Z}_2$ factor of the Klein symmetry of the Majorana mass matrix is accidental.

The field content encompasses all Standard Model fields, an additional second Higgs boson such that there are two Higgs doublets $h_u = (\mathbf{1}, \mathbf{2}, 1/2)$ and $h_d = (\mathbf{1}, \mathbf{2}, -1/2)$ like, for example, in the MSSM, and three flavon fields φ_e, φ_ν and ξ. Their representations with respect to A_4 and charges under an additional abelian $\mathbb{Z}_4$ symmetry are displayed in Table III.5. The terms responsible for lepton masses after flavour and electroweak symmetry breaking

8 Note that the basis used in the original reference is different from the one employed here.

are [9, 10]

$$\begin{aligned}\mathcal{L}_m \coloneqq & \frac{h_e}{\Lambda} h_d\, e^c\, (\varphi_e \otimes l)_{\mathbf{1}} + \frac{h_\mu}{\Lambda} h_d\, \mu^c\, (\varphi_e \otimes l)_{\mathbf{1}'} + \frac{h_\tau}{\Lambda} h_d\, \tau^c\, (\varphi_e \otimes l)_{\mathbf{1}''} \\ & + \frac{\lambda_1}{\Lambda \Lambda_\nu} \left\{ [(l\, h_u) \otimes (l\, h_u)]_{\mathbf{3}_\mathrm{s}} \otimes \varphi_\nu \right\} + \frac{\lambda_2}{\Lambda \Lambda_\nu} \left[(l\, h_u) \otimes (l\, h_u) \right]_{\mathbf{1}} \xi\,.\end{aligned} \tag{3.1}$$

Here h_f and λ_i are dimensionless coupling constants, Λ the flavour scale and Λ_ν the, possibly identical, See-saw scale. The general structure of the mass terms is common to all flavour models with discrete non-abelian symmetries. There are usually several flavon fields which are not charged with respect to the Standard Model gauge group but with respect to the flavour group. Some of these flavons should transform in higher-dimensional representations of the flavour group to generate a non-trivial mixing structure. Further, either leptons or anti-leptons or both reside in higher-dimensional representations. This combination yields relations among the mass terms of different generations that are, at least to a certain degree, predicted by the group structure. An additional abelian symmetry like the $\mathbb{Z}_4$ in the example is used to forbid unwanted couplings, a method which is so common in flavour model building that there is the danger of a proliferation of such symmetries. Due to the finite order of these symmetries, one has to be careful that allowed higher-order terms do not spoil the desired structure.

After performing the contractions in (3.1) according to the rules of Section A.1.1 and inserting the Higgs vacuum expectation values, see Table III.5, one arrives at the following mass matrices for charged leptons and neutrinos:

$$m_e = \frac{v_d}{\sqrt{3}\Lambda} \begin{pmatrix} h_e \langle\varphi_{e,1}\rangle & h_e \langle\varphi_{e,3}\rangle & h_e \langle\varphi_{e,2}\rangle \\ h_\mu \langle\varphi_{e,2}\rangle & h_\mu \langle\varphi_{e,1}\rangle & h_\mu \langle\varphi_{e,3}\rangle \\ h_\tau \langle\varphi_{e,3}\rangle & h_\tau \langle\varphi_{e,2}\rangle & h_\tau \langle\varphi_{e,1}\rangle \end{pmatrix}, \tag{3.2a}$$

$$\begin{aligned} m_\nu = & \frac{2\, v_u^2}{3 \Lambda \Lambda_\nu} \cdot \\ & \begin{pmatrix} \left(\sqrt{3}\lambda_2 \langle\xi\rangle + \sqrt{2}\lambda_1 \langle\varphi_{\nu,1}\rangle\right) & -\frac{1}{\sqrt{2}}\lambda_1 \langle\varphi_{\nu,3}\rangle & -\frac{1}{\sqrt{2}}\lambda_1 \langle\varphi_{\nu,2}\rangle \\ -\frac{1}{\sqrt{2}}\lambda_1 \langle\varphi_{\nu,3}\rangle & \sqrt{2}\lambda_1 \langle\varphi_{\nu,2}\rangle & \sqrt{3}\lambda_2 \langle\xi\rangle - \frac{1}{\sqrt{2}}\lambda_1 \langle\varphi_{\nu,1}\rangle \\ -\frac{1}{\sqrt{2}}\lambda_1 \langle\varphi_{\nu,2}\rangle & \sqrt{3}\lambda_2 \langle\xi\rangle - \frac{1}{\sqrt{2}}\lambda_1 \langle\varphi_{\nu,1}\rangle & \sqrt{2}\lambda_1 \langle\varphi_{\nu,3}\rangle \end{pmatrix}. \end{aligned} \tag{3.2b}$$

Inspecting these mass matrices it is immediately clear that one of the crucial points of this type of model is the alignment of the flavon vacuum expectation values. If the triplet VEVs in this model were completely arbitrary, no structure would be recognisable in the mass matrices. With the specific choice of Table III.5, however, one obtains

$$m_e = \frac{v_d\, v'}{\sqrt{3}\Lambda} \begin{pmatrix} h_e & 0 & 0 \\ & h_\mu & 0 \\ 0 & 0 & h_\tau \end{pmatrix}, \tag{3.3a}$$

$$m_\nu = \frac{v_u^2}{3 \Lambda \Lambda_\nu} \begin{pmatrix} a + 2\,d & -d & -d \\ -d & 2\,d & a - d \\ -d & a - d & 2\,d \end{pmatrix}, \tag{3.3b}$$

where the abbreviations $a \coloneqq 2\sqrt{3}\lambda_2\, w$ and $d \coloneqq \sqrt{2}\lambda_1\, v$ are used. As the charged lepton mass matrix is already diagonal, which is one reason for the present choice of A_4 basis, the

mass eigenstates coincide with the flavour eigenstates up to phase changes, which can be absorbed into the charged lepton singlet fields. Three couplings are involved in determining the three mass values; thus, there is no prediction but one can fit the correct values. The model as presented so far does not provide any reason for the hierarchy among the charged lepton masses, a deficit which is shared by most models with discrete non-abelian flavour symmetries. However, this could be remedied here by introducing an additional Froggatt–Nielsen symmetry acting on the charged lepton singlets as they are singlets under the flavour symmetries [9].

With a diagonal charged lepton mass matrix, the PMNS matrix is the same as U_ν up to possible phases. Computing the lepton mixing matrix, it turns out that

$$U_{\text{PMNS}} = U_\nu = \begin{pmatrix} \sqrt{\frac{2}{3}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \operatorname{diag}\left(\mathrm{e}^{\mathrm{i}\arg(a+3d)/2}, \mathrm{e}^{\mathrm{i}\arg(a)/2}, \mathrm{e}^{\mathrm{i}\arg(-a+3d)/2}\right), \tag{3.4}$$

i.e. U_{PMNS} is a tri-bi-maximal matrix, compare equation (2.4), with additional Majorana phases. One particular feature of this model is that the mixing angles do not depend on any couplings.[9]

The neutrino masses are

$$m_{\nu_i} = \frac{v_u^2}{3\Lambda\Lambda_\nu} \cdot \begin{cases} |a+3d|\,, & i=3\,, \\ |a|\,, & i=2\,, \\ |-a+3d|\,, & i=1\,. \end{cases} \tag{3.5}$$

Assuming real couplings, which can be obtained by imposing a CP symmetry, see also Chapter VII, the fact that there are only two couplings involved in three mass values leads to a prediction of the absolute mass scale from the mass differences [9].

Before concluding the discussion of the A_4 example model, corrections to the first order mixing pattern obtained so far shall be mentioned. Since the Lagrangian contains effective operators of orders five and six, there is no good reason for stopping the expansion at any fixed order. Indeed, one should take into account all higher-order terms that are consistent with the symmetries of the theory. These terms can be expected to perturb the mixing matrix away from the tri-bi-maximal pattern without destroying the picture completely because the perturbations are suppressed by additional factors of vacuum expectation values over fundamental or See-saw scale. Such perturbations are welcome, for the angles of tri-bi-maximal mixing deviate from the measured values, most notably $\theta_{13} \approx 8.5° \neq 0$. Usually, only higher-order terms for the potential (or superpotential for supersymmetric models) are investigated [9]. However, there are also operators which, after flavour symmetry breaking, change the normalisation of kinetic terms of matter fields (Kähler potential terms in supersymmetric models); thus, they influence the mixing angles via the additional re-normalisation of fields to be performed. These corrections are discussed in detail in Chapter V. An important difference between these two types of higher-order terms is that superpotential terms can be forbidden by additional abelian shaping symmetries while this is impossible for certain corrections to the kinetic terms. A further correction that should be taken into account is the renormalisation group (RG) running of mixing parameters as they are not RG invariant [93–95].

9 This feature is sometimes called ‘form-diagonalisability’.

III.4 Critical assessment of discrete non-abelian flavour symmetries

As seen in this chapter, the flavour structure of the Standard Model clearly asks for a more fundamental explanation. Popular candidates for a solution to this flavour puzzle are models with discrete non-abelian flavour symmetries. Models with such symmetries can, in principle, generate a non-trivial mixing structure, no Goldstone bosons are generated in the process of flavour symmetry breaking, and the symmetries can be protected from gravitational violation. Many models built within this framework so far predict one of the three mixing structures called tri-bi-maximal mixing, bi-maximal mixing and golden ratio mixing, whose mixing angles are not too far from experimental values. However, higher-order corrections have to be taken into account both to obtain robust predictions and to arrive at realistic values for the mixing parameters.

Although aesthetically appealing, model building with discrete flavour symmetries has to face some criticism. One particular reason is the ambiguity enjoyed by the models coming from the choice of symmetry and field content. There is clearly an infinite number of finite non-abelian groups, even when restricting the discussion to groups with three-dimensional irreducible representations, cf. e.g. the $\Delta(3\,n^2)$ series of $\mathrm{SU}(3)$ subgroups. Usually, the choice of group is only based on arguments like simplicity and minimal size, leading to groups like the tetrahedral group A_4 used in the example model.

Even after choosing a group, there is still the possibility to freely introduce fields in arbitrary irreducible representations. Of course, one would again try to be as economical as possible, but this is a rather vague requirement. The situation is improved if one obtains the discrete group by spontaneously breaking a continuous (gauge) symmetry because one is then restricted to a field content that can arise from the breaking, see Chapter VI.

Another type of uncertainty enters the model building process when imposing, rather than actually deriving, the VEV alignment of the flavons because then there is no guarantee that the chosen alignment is physical. In many (especially supersymmetric) models the seemingly sharp line between deriving a VEV alignment from a potential and inserting it by hand is blurred by the introduction of many additional driving fields, cf. [10, 37]. Using this mechanism, one can, in principle, write down potentials with arbitrary minima with great ease; however, this is at the expanse of a large number of additional abelian shaping symmetries and driving fields, cf. e.g. the models [27, 96, 97].

The situation is improved in string model building, where discrete flavour groups can naturally arise [62, 98–100]. While it is not yet entirely clear which classes of finite groups one can obtain from string constructions, it is impossible to pick a group at will. Moreover, the field content of the model is set from the beginning and cannot be changed, completely removing this ambiguity. Nevertheless, as there is a huge number of string vacua, it remains very difficult to make definite predictions.

IV Anomaly-safe discrete groups

Usually, symmetries of the action defining a theory are assumed also to be symmetries at the quantum level, i.e. symmetries of the generating functional of the corresponding quantum field theory. It is, of course, well known that this is not always the case [101, 102]. The breaking of a classical symmetry at the quantum level is called anomaly and the symmetry is said to be anomalous. This possibility is not restricted to continuous symmetries but can equally affect discrete symmetries such as the ones discussed in the previous section [61]. Such symmetries are then violated at least non-perturbatively. Hence, checking whether a discrete symmetry is anomaly free is crucial for its phenomenological understanding. This becomes particularly acute if the symmetry is to be embedded into a gauge symmetry at high energies to shield it from gravitational violation. In this case it has to be anomaly free because, otherwise, this high-energy gauge symmetry would have to be anomalous as well, rendering it inconsistent.

For abelian finite groups, anomaly constraints were first derived from the spontaneous breaking of $\mathrm{U}(1)$ symmetries [103–105]. It was shown in [106, 107], however, that discrete anomalies can also be derived from the transformation of the path integral measure used first by Fujikawa [108, 109] for continuous symmetries. This derivation also shows clearly that the only anomaly constraints one has to consider are of the form $G - L - L$ where L denotes the (Lie) gauge group of the theory, i.e. there is no $G - G - G$ anomaly for global symmetries G (including discrete G). Nonetheless, it is possible to consider the constraints obtained from embedding the discrete group into a continuous anomaly-free symmetry [110, 111]. The resulting restrictions on the symmetry are then, in general, stronger than strictly needed for anomaly freedom. Thus, the path integral method is employed in the following to determine the anomalies of discrete groups and to show which kinds of groups are anomaly free regardless of the details of a specific model.

First, the anomaly conditions on discrete groups derived from the transformation of the path integral measure are reviewed, and it is shown that the path integral measure transforms in a well-defined one-dimensional representation of the discrete group. Based on this argument it is easy to see that perfect groups, and thus also simple groups, are anomaly free, whereas all other groups may suffer, in general, from anomalies. Moreover, the argument shows that such anomalies always can consistently be cancelled by a discrete Green–Schwarz mechanism [41, 64, 112]. Particular care is taken of the normalisation of the gauge group Dynkin indices, and it is shown that orthogonal and exceptional gauge groups are somewhat less prone to anomalies than unitary and symplectic groups, a fact that has not been noted before.

* Some of the results presented in this chapter have already been communicated in [5].

L	SU(N)	Sp($2N$)	SO(N)	G_2	F_4	E_6	E_7	E_8
$\ell(\boldsymbol{F}_L)$	1/2	1/2	1	1	3	3	6	30

Table IV.1: Dynkin indices of the fundamental representations of the simple compact Lie groups L using the conventions of Bernard et al. [114].

IV.1 Anomalies of discrete groups

The theory under consideration shall be defined by a Lagrangian which is invariant under a discrete symmetry G and a gauged compact simple Lie group L.[1] Moreover, let Ψ be a multiplet of Dirac fermions transforming in a representation $\boldsymbol{r}$ of L. Consider now a chiral transformation of the left-handed part $\Psi_L := P_L\,\Psi$ of the multiplet Ψ, which is assumed to transform in a unitary representation $\boldsymbol{R}$ of G,

$$\Psi_L \mapsto \rho_{\boldsymbol{R}}(g)\,\Psi_L\,. \tag{1.1}$$

As group representation matrices are invertible, any $\rho_{\boldsymbol{R}}(g)$ has a matrix logarithm $\ln\rho_{\boldsymbol{R}}(g)$ such that

$$\rho_{\boldsymbol{R}}(g) = \mathrm{e}^{\ln\rho_{\boldsymbol{R}}(g)}\,, \tag{1.2}$$

cf. e.g. [113]. This logarithm is, of course, not unique, but it turns out that its use is only necessary at intermediate steps; it completely drops out in the final results. Hence, any specific choice of logarithm is permitted.

The transformation of the path integral measure is then (cf. [107])

$$\mathcal{D}\Psi\,\mathcal{D}\overline{\Psi} \mapsto \mathcal{D}\Psi\,\mathcal{D}\overline{\Psi}\,\mathcal{J}_\Psi := \mathcal{D}\Psi\,\mathcal{D}\overline{\Psi}\,\exp\left\{\mathrm{tr}\,(\ln\rho_{\boldsymbol{R}}(g))\cdot\ell(\boldsymbol{r})\cdot\int \mathrm{d}^4x\,\frac{1}{16\,\pi^2}\,F_{\mu\nu,a}\,\tilde{F}_a^{\mu\nu}\right\}. \tag{1.3}$$

The definition of the field strength tensor $F_{\mu\nu} = F_{\mu\nu,a}\,T^a$ used is $F_{\mu\nu} := \mathrm{i}\,[D_\mu, D_\nu]$ with the gauge covariant derivative $D_\mu := \partial_\mu - \mathrm{i}\,A_\mu = \partial_\mu - \mathrm{i}\,A_{\mu,a}\,T^a$. Further, the dual field strength is normalised as $\tilde{F}^{\mu\nu} := \frac{1}{2}\,\varepsilon^{\mu\nu\rho\sigma}\,F_{\rho\sigma}$. Finally, T^a denotes the generators of the Lie algebra of L, whose normalisation is chosen according to the convention of Bernard et al. [114]. Hence, the longest root of the Lie algebra of L has length one or, equivalently, the Dynkin index

$$\delta^{ab}\;\ell(\boldsymbol{r}) := \mathrm{tr}\left(\boldsymbol{r}(T^a)\,\boldsymbol{r}(T^b)\right) \tag{1.4}$$

evaluated in the adjoint representation, $\boldsymbol{r} = \mathbf{adj}$, equals the dual Coxeter number of the algebra (cf. e.g. [115]). The resulting Dynkin index $\ell(\boldsymbol{F}_L)$ for the fundamental representations $\boldsymbol{F}_L$ of the simple compact Lie groups L, which are the representations of smallest dimension, are shown in Table IV.1. Dynkin indices for all other representations are integer multiples of these values.

In contrast to the continuous case, where the group transformation parameters can take arbitrary values, the normalisation is crucial for the discrete case. The reason is that the index theorems (cf. e.g. [116]) imply that the Pontryagin index

$$P := \int \mathrm{d}^4x\,\frac{1}{32\,\pi^2}\,F_{\mu\nu,a}\,\tilde{F}_a^{\mu\nu} \tag{1.5}$$

1 The discussion can be repeated for abelian groups and gravity.

is an integer for any gauge field configuration in the chosen normalisation [114, 117]. In a different normalisation it would, of course, still be a topological charge, but it might take values in, for example, $\mathbb{Z}/2$ or $2\,\mathbb{Z}$ instead. For the chosen normalisation, however, it was shown in [114], using the theorem that any mapping from S_3 into a simple Lie group L can be deformed to a mapping into an $\mathrm{SU}(2)$ subgroup of L [118], that, varying the gauge field configuration, precisely all integers are assumed by P. This normalisation issue was not properly taken into account in previous studies of non-abelian discrete anomalies using the path integral [106, 107] and leads to differences in anomaly conditions for orthogonal and exceptional groups compared to unitary and symplectic groups, see Section IV.2 below.

Using this abbreviation and the identity

$$\det \mathrm{e}^{A} = \mathrm{e}^{\operatorname{tr} A} \tag{1.6}$$

for any complex square matrix A, the path integral transformation (1.3) can be rewritten to

$$\mathcal{D}\Psi\,\mathcal{D}\overline{\Psi}\,\mathcal{J}_{\Psi} = \mathcal{D}\Psi\,\mathcal{D}\overline{\Psi}\,\det\left(\rho_{\boldsymbol{R}}(g)\right)^{2\,\ell\,(\boldsymbol{r})\,\cdot\,P}. \tag{1.7}$$

Note that as $\boldsymbol{R}$ is assumed to be unitary, which is no restriction for finite discrete groups, see Theorem 7, the determinant lies on the unit circle in $\mathbb{C}$. Moreover, since the determinant is a group homomorphism from $\mathrm{GL}(n,\mathbb{C})$ to $\mathrm{GL}(1,\mathbb{C}) = \mathbb{C}^{\times}$, the composition of group homomorphisms $(\det \circ \boldsymbol{R})$ is a one-dimensional representation of G. Using the additional information that $2\,\ell\,(\boldsymbol{R})\cdot P$ is an integer and that integer powers of one-dimensional representations are themselves one-dimensional representations, one concludes that the path integral measure transforms in a one-dimensional representation of the discrete group G.[2] This fact is exploited in several ways in the following section.

IV.2 Anomaly-safe discrete groups

Going back to the physics application, the symmetry G is anomaly free if and only if the product of the path integral measures of all fields f transforms trivially, i.e. if and only if[3]

$$\prod_{f} \det\left(\rho_{\boldsymbol{R}^f}(g)\right)^{2\,\ell\,(\boldsymbol{r}^f)\,\cdot\,P} = 1\,, \qquad \forall\, P \in \mathbb{Z}\,, \forall\, g \in G\,. \tag{2.1}$$

A group G can be said to be anomaly safe if it does not suffer from anomalies independently of the specific field content and of the gauge symmetries present. This is true if

$$\det\left(\rho_{\boldsymbol{R}_i}(g)\right) = 1\,, \qquad \forall\, g \in G\,, \tag{2.2}$$

for all irreducible representations $\boldsymbol{R}_i$ since the minimal non-trivial P is one and the minimal Dynkin index is $1/2$, see again Table IV.1. This is, by the arguments outlined above, equivalent to the requirement that G shall not have any non-trivial one-dimensional representation at all.

As stated in Chapter II, the one-dimensional representations of G are in one-to-one correspondence with the representations of its Abelianisation $A(G)$, see Definition 13 and

2 The statements of the last two sentences are true since $\det A\,B = \det A \cdot \det B$ and $(a\,b)^n = a^n\,b^n$ for $a,\, b \in \mathbb{C}$.

3 For a discussion using the more common notion of anomaly-coefficients, yielding modular equations for the sum of the $\operatorname{tr}\left(\ln \rho_{\boldsymbol{R}}(g)\right)$ for all fields, see [5].

Theorem 6. Assume from now on that the Abelianisation is finite, which is clear for finite G but can also happen for infinite groups as, for example, $\mathrm{SL}(2,\mathbb{Z})$. As an abelian group, $A(G)$ has $|A(G)|$ inequivalent irreducible representations, i.e. anomaly-safe groups have $|A(G)| = 1$.[4] Groups with trivial Abelianisation, i.e. groups which equal their commutator subgroup, are called perfect groups, see Definition 14. This shows that the notion of perfect group coincides with the definition of anomaly-safe group used here.[5]

It follows from Theorem 1 that all non-abelian simple groups are perfect. These groups are the groups into which all finite groups can be decomposed using the composition series [120]. Examples are all alternating groups A_n with $n \geq 5$, the projective special linear groups $\mathrm{PSL}(n,k)$ with $n \geq 2$ over finite fields k (without $\operatorname{char} k \leq 3$ while $n = 2$) and other classical and exceptional finite groups of Lie type [120]. Among them especially A_5, which can yield golden ratio mixing when applied to neutrino model building [84], and $P\mathrm{SL}(2,7) = \Sigma(168)$, which can yield tri-bi-maximal mixing [121], have been used in model building. For more information on these groups, see [57], and for recent model building approaches utilising them, see [122–124].

However, since perfect groups are not the same as non-abelian simple groups, there are also non-abelian, non-simple perfect groups. Examples are the special linear groups $\mathrm{SL}(n,k)$ with $n \geq 2$ over finite fields k (without $\operatorname{char} k \leq 3$ while $n = 2$) [120] and semi-direct products of perfect groups. The latter can be seen because any element of a semi-direct product can be written as the product of one group element of each factor, see Definition 16; hence, it can be written as the product of commutator elements, i.e. every group element is an element of the commutator subgroup. This includes, as the trivial example of a semi-direct product, also direct products of perfect groups. Note that the semi-direct product of two simple groups is perfect but not simple since one of the two factors is a non-trivial normal subgroup of the product.

Sometimes in model building, one is already sure about the symmetries, or at least gauge symmetries, of a model, although the field content has not been fixed completely. In this case, it turns out that the definition of anomaly-safe groups given above can be too strong. The reason is that only for $\mathrm{SU}(N)$ and $\mathrm{Sp}(2N)$ the smallest Dynkin label is $1/2$; for $\mathrm{SO}(N)$, for example, it is one. Hence, given $\mathrm{SO}(N)$ as gauge group, the exponent in equation (1.7) is always an even integer instead of just any integer. Therefore, groups whose one-dimensional representations only have ± 1 as image are free of anomalies with respect to $\mathrm{SO}(N)$ gauge groups. An important example are the symmetric groups (for their representations, cf. [57]), which are thus free of $\mathrm{S}_n - \mathrm{SO}(N) - \mathrm{SO}(N)$ anomalies and, in fact, free of $\mathrm{S}_n - L - L$ anomalies for L not $\mathrm{SU}(N)$ and $\mathrm{Sp}(2N)$. $\mathrm{S}_n - \mathrm{SU}(N) - \mathrm{SU}(N)$ anomalies, however, may exist.

More generally, a discrete group G is free of anomalies with respect to a given gauge group L irrespectively of the field content if and only if

$$\det\left(\rho_{\boldsymbol{R}_i}(g)\right)^{2\,\ell(\boldsymbol{F}_L)} = 1\,, \qquad \forall\, g \in G\,, \qquad \forall\, i \tag{2.3}$$

for the fundamental representation $\boldsymbol{F}_L$ of L and all irreducible representations $\boldsymbol{R}_i$ of G since all other Dynkin indices are integer multiples of $\ell(\boldsymbol{F}_L)$. This condition is certainly fulfilled if

$$\frac{2\,\ell(\boldsymbol{F}_L)}{|A(G)|} \in \mathbb{Z}\,. \tag{2.4}$$

4 The sum of the squares of the dimensions over all inequivalent irreducible representations of a finite group equals the order of the group. Since for abelian groups the orders are all one, the stated result follows.

5 The fact that perfect groups are anomaly free was first realised in [119] using anomaly coefficients.

To see this, note that the order of $A(G)$ is an upper bound on the orders of its group elements. These are, in turn, by the correspondence of one-dimensional representations of G with the representations of $A(G)$, the same as the powers needed for (2.3) to be true. This is already sufficient for the case of the symmetric groups because $[\mathrm{S}_n, \mathrm{S}_n] = \mathrm{A}_n$ and $\mathrm{S}_n/\mathrm{A}_n = \mathbb{Z}_2$ [21]. Also the case of completely anomaly-safe groups can be derived immediately because perfect groups have $A(G) = 1$.

However, the argument can still be refined for more complicated Abelianisations. Since any finite abelian group can be written as the direct product of cyclic groups with powers of prime numbers as orders, see Theorem 2,

$$A(G) = \bigtimes_{i,j} \mathbb{Z}_{p_i^{n^{i,j}}} \tag{2.5}$$

for some prime numbers p_i and natural numbers $n^{i,j}$. The maximal order of an element of $A(G)$ is thus $\prod_i \max_j n^{i,j}$, which allows for a refinement of (2.4) to a necessary and sufficient condition. In fact, a discrete group G is anomaly free with respect to a gauge group L irrespectively of the field content if and only if

$$\frac{2\,\ell\,(\boldsymbol{F}_L)}{\prod_i \max_j n^{i,j}} \in \mathbb{Z}\,. \tag{2.6}$$

IV.3 Further comments and conclusion of the chapter

It was shown that perfect groups and, therefore, non-abelian simple groups are anomaly safe, i.e. that they are not anomalous irrespective of gauge group and field content. If one abandons the first condition and specifies the gauge group, the results (2.4) and (2.6) show that some discrete groups are anomaly free irrespective of the field content for $\mathrm{SO}(N)$ or exceptional gauge groups but, in general, anomalous with respect to $\mathrm{SU}(N)$ and $\mathrm{Sp}(2N)$. This shows that theories with gauge group $\mathrm{SO}(N)$ or exceptional gauge groups are somehow less prone to anomalies than theories with $\mathrm{SU}(N)$.

The discussion is also applicable to infinite discrete groups like $\mathrm{SL}(2,\mathbb{Z})$, although, of course, statements involving the order of the Abelianisation only make sense if this is a finite number. Note, however, that one has to make sure that the assumption of a unitary transformation, i.e. equation (1.1), is fulfilled. For example, the T-duality transformation of string theory, which is known to be anomalous [125, 126], does not fall into this class in its usual formulation (cf. e.g. [127]), and it is not clear whether one can choose a basis such that the present discussion can be applied.

Some results stay even true for mixed anomalies of continuous groups. In fact, the derivation of (1.7) is valid for $L' - L - L$ anomalies, where L and L' are different Lie groups (not necessarily structurally, but as symmetries of the theory). The result can then be used, for example, to show that $\mathrm{SU}(N) - \mathrm{SU}(M) - \mathrm{SU}(M)$ anomalies vanish by virtue of the fact that $\mathrm{SU}(N)$ is perfect [23].[6] The structure of $L - L - L$ anomalies, i.e. of cubic anomalies, however, is completely different, and the presented results cannot be applied to this case.

Additionally, the present discussion allows a simple understanding of the fact derived in [119] that, whenever a discrete symmetry is anomalous, one may employ a so-called discrete

6 Note that it is not sufficient to observe that $\mathrm{SU}(N)$ is generated by unitary matrices of dimension N with determinant one because there could, in principle, be other representations that do not have determinant one for all elements.

Green–Schwarz mechanism to cancel it [41, 64, 112]. The basic idea of this mechanism is that there is a field, called axion, that couples to the $F_{\mu\nu}\tilde{F}^{\mu\nu}$ term in the Lagrangian and shifts under the given discrete symmetry in such a way that the anomaly is exactly cancelled. The anomaly only returns as soon as the axion acquires a vacuum expectation value. An obstruction would occur if there were no transformation behaviour for the axion to achieve the cancellation. However, since it was shown that the path integral measure transforms in a proper one-dimensional representation, the axion just has to transform as the phase of the complex conjugate representation. This requirement is completely consistent for any discrete group and thus settles the discussion.

V Kinetic term corrections to neutrino mixing

As outlined in Section III.2, one can make a good case for models with discrete non-abelian flavour symmetries to be (part of) the explanation of the lepton flavour structure. In particular, the neutrino mixing matrix as determined by experiment comes reasonably close to several highly symmetric types of mixing matrices, e.g. to the tri-bi-maximal matrix (III.2.4), even though most of them predict a mixing angle θ_{13} of zero in contrast to the measured value of about 8.5°. However, to be precise, the prediction of, for example, tri-bi-maximal mixing by the A_4 model reviewed in Section III.3 is only true at lowest non-trivial order. Since these models are in the framework of effective field theory, i.e. their Lagrangians are non-renormalisable, there is no reason to cut off the expansion in $1/\Lambda$ at any fixed order, where Λ is the scale at which the effective theory breaks down due to new physics. Hence, any such model can be expected to receive higher-order corrections that perturb the mixing matrices away from their symmetric lowest-order structures.

On the one hand, this is desirable because it might explain the deviations, e.g. why $\theta_{13} \neq 0$. On the other hand, it might prove disastrous if the good features of a model are lost due to the higher-order contributions. Moreover, at higher order, there is usually a proliferation of couplings because more and more terms invariant under all symmetries can be written down. If their effect is too large, this can diminish the predictive power of a model altogether unless there is a way to control these couplings. This is particularly pressing in flavour models because flavon fields are often assumed to attain rather large vacuum expectation values up to the order of a tenth of the new physics scale.

Corrections to the (super-) potential are often considered, cf. e.g. [9, 10] for the A_4 model, and they are in a certain way under control because it is usually possible to forbid dangerous terms by additional abelian shaping symmetries. In contrast to that, terms changing the normalisation of matter fields are ignored in most analyses, although it has long been known that they exist [128, 129]. They arise if a flavon field, or any field obtaining a vacuum expectation value, couples to the kinetic terms of matter fields, e.g. of the neutrinos. A comparison with experimental results like mixing angles, however, only makes sense for a theory with canonically normalised fields, and during the process of re-normalising the fields the mixing structure is changed [130–133]. Such changes occur because, as detailed in Section III.2, the flavour symmetry has to be fully broken for a realistic spectrum to arise, and, hence, the mixing parameters are not protected by the symmetry any more. This is also reflected in the fact that there is a non-trivial renormalisation group running of the mixing parameters [94, 95].

* Some of the results presented in this chapter have already been communicated in [1, 2].

The canonical normalisation effects are discussed here using a supersymmetric terminology. The results, however, are also applicable to non-supersymmetric models. This is explained after briefly reviewing the definition of the Kähler potential, which contains the kinetic terms in supersymmetric theories, in the next section. Afterwards, the effects of additional Kähler potential terms on the mass matrices are discussed in Section V.2. In the subsequent section, analytical formulas are derived that relate additional contributions to the Kähler metric, or to the kinetic terms in non-supersymmetric models, directly to changes in the mixing angles.[1] These formulas are completely independent of the specific model and only depend on the mixing parameters and masses as determined before taking into account the corrections. Furthermore, the MATHEMATICA package `KaehlerCorrections` is presented, in which these formulas are implemented. It is publicly available online.[2]

Using these analytical formulas, the A_4 model of Section III.3 and a further flavour model with a T′ symmetry are analysed with respect to possible kinetic term corrections. Thus, it is shown that, in contrast to earlier claims in the literature [134], the changes of the mixing angles are not small and that such corrections must be taken into account when determining the predictions of a model. Moreover, results for general contributions to the kinetic terms for tri-bi-maximal and bi-maximal mixing are presented in Section V.4.3.

For supersymmetric models, furthermore, the implications of Kähler corrections for the alignment of vacuum expectation values are considered, and some comments are made on the possibility of constricting Kähler potential couplings using experimental results on flavour changing neutral currents.

V.1 The Kähler potential

No general introduction to supersymmetry is given here because the effects to be discussed below can be understood without this knowledge. For introductions to SUSY, cf. [135–138]. Here only the notions of Kähler potential and superpotential are reviewed and the connection to non-supersymmetric models is made.

A supersymmetric theory is determined by three functions of superfields:

(i) the superpotential W, which is a holomorphic function of chiral superfields Φ;

(ii) the gauge kinetic function f_{ab}, which is also a holomorphic function of chiral superfields and which has two indices a and b running over the adjoint representation of the gauge group;

(iii) the Kähler potential K, which is a real function of the chiral superfields and their complex conjugates multiplied with the gauge connection matrix $\mathrm{e}^{-2\,V_a\,T^a}$.

The full Lagrangian is then [138]

$$\mathcal{L} = \int \mathrm{d}^2\theta\,\mathrm{d}^2\bar{\theta}\,K(\Phi,\,\Phi^\dagger\,\mathrm{e}^{-2\,V}) + \int \mathrm{d}^2\theta\left[\frac{1}{4}f_{ab}(\Phi)\,\mathcal{W}^a\,\mathcal{W}^b + W(\Phi) + \mathrm{h.\,c.}\right] \tag{1.1}$$

where $\mathcal{W}^a$ are the gauge superfields.

1 Note that the whole chapter focuses on Majorana neutrinos.
2 http://einrichtungen.ph.tum.de/T30e/codes/KaehlerCorrections

To obtain kinetic terms for the fermion field ψ, its scalar superpartner φ and the auxiliary field F residing in a chiral supermultiplet Φ, one sets the Kähler potential to

$$K(\Phi,\, \Phi^\dagger\, \mathrm{e}^{-2\,V}) = \Phi^\dagger\, \mathrm{e}^{-2\,V}\, \Phi\,. \tag{1.2}$$

Neglecting the gauge boson contributions because they do not affect the discussion, the resulting kinetic terms are precisely the desired canonically normalised ones [138],

$$\mathcal{L}_{\text{kinetic}} = \int \mathrm{d}^2\theta\, \mathrm{d}^2\bar\theta\, \Phi^\dagger\Phi = (\partial_\mu\varphi^*)\,(\partial^\mu\varphi) + \frac{\mathrm{i}}{2}\,\psi^\dagger\,\bar\sigma^\mu\,\partial_\mu\psi - \frac{\mathrm{i}}{2}\,(\partial_\mu\psi^\dagger)\,\bar\sigma^\mu\,\psi + F^*F\,. \tag{1.3}$$

Interactions are usually introduced by adding a non-trivial superpotential. In fact, after integrating out the auxiliary fields [138]

$$S = \int \mathrm{d}^4x \left[(\partial_\mu\varphi^*)\,(\partial^\mu\varphi) + \mathrm{i}\,\psi^\dagger\,\bar\sigma^\mu\,\partial_\mu\psi - \underbrace{\left|\frac{\partial W}{\partial\Phi}(\varphi)\right|^2}_{\text{scalar potential } V(\varphi,\,\varphi^*)} - \left(\frac{1}{2}\frac{\partial^2 W}{\partial\Phi^2}(\varphi)\,\psi^2 + \text{h. c.}\right)\right], \tag{1.4}$$

i.e. the superpotential determines the form of the potential. However, there is no reason to restrict the Kähler potential to the canonical one shown in equation (1.2). In fact, higher-order Kähler potential terms are generated, for example, in string theory and are on equal footing with superpotential terms. For an arbitrary Kähler potential, the superspace integral over K is

$$\begin{aligned}\mathcal{L} &\supset \int \mathrm{d}^2\theta\, \mathrm{d}^2\bar\theta\, K(\Phi,\, \Phi^\dagger\, \mathrm{e}^{-2\,V}) \\ &= \mathcal{K}^{ij}(\varphi,\,\varphi^*)\left((\partial_\mu\varphi_i^*)\,(\partial^\mu\varphi_j) + \frac{\mathrm{i}}{2}\,\psi_i^\dagger\,\bar\sigma^\mu\,\partial_\mu\psi_j - \frac{\mathrm{i}}{2}\,(\partial_\mu\psi_i^\dagger)\,\bar\sigma^\mu\,\psi_j + F_i^*F_j\right) + \cdots\,,\end{aligned} \tag{1.5}$$

where only kinetic terms are displayed and where

$$\mathcal{K}^{ij}(\varphi,\,\varphi^*) \coloneqq \frac{\partial^2 K}{\partial\Phi_i^\dagger\,\partial\Phi_j}(\varphi,\,\varphi^*) \tag{1.6}$$

is the Hermitian, field-dependent Kähler metric. The canonical Kähler metric is therefore

$$\mathcal{K}^{ij}(\varphi,\,\varphi^*) = \delta^{ij}\,. \tag{1.7}$$

Any Kähler potential should contain (1.2) as a subset such that the Lagrangian includes the usual kinetic terms, but there may be additional terms of higher mass dimension.

In principle, these additional terms are just interaction terms similar, though structurally different, to the ones contained in the superpotential. Indeed, for example, the scalar potential changes to

$$\begin{aligned}V(\varphi,\,\varphi^*) = {}& \left(\mathcal{K}^{ij}(\varphi,\,\varphi^*)\right)^{-1}\,\frac{\partial W^*}{\partial\Phi_i^\dagger}(\varphi^*)\,\frac{\partial W}{\partial\Phi_j}(\varphi) \\ &+ \frac{1}{2}\,\left(\mathrm{Re}\,f_{ab}(\varphi)\right)^{-1}\,\mathrm{Re}\left(\frac{\partial K}{\Phi_i}(\varphi,\varphi^*)\cdot(T^a\,\varphi)_i\right)\,\mathrm{Re}\left(\frac{\partial K}{\Phi_j}(\varphi,\varphi^*)\cdot(T^a\,\varphi)_j\right)\end{aligned} \tag{1.8}$$

for an arbitrary Kähler potential.

However, these interactions can have the additional effect of changing the normalisation of fields. The effective kinetic terms are determined by the Kähler metric evaluated at the vacuum expectation values of all fields,

$$\hat{\mathcal{K}}^{ij} := \mathcal{K}^{ij}(\langle\varphi\rangle, \langle\varphi^*\rangle)\,. \tag{1.9}$$

Using this matrix, the kinetic terms read

$$\mathcal{L}_{\text{kinetic}} = \hat{\mathcal{K}}^{ij}\left((\partial_\mu\varphi_i^*)\,(\partial^\mu\varphi_j) + \mathrm{i}\,\psi_i^\dagger\,\bar{\sigma}^\mu\,\partial_\mu\psi_j\right)\,. \tag{1.10}$$

Depending on the interaction terms and VEVs, a non-canonical Kähler potential can thus have the effect of changing the normalisation of the kinetic terms due to $\hat{\mathcal{K}} \neq \mathbb{1}$. This is precisely what happens in flavour models like the one presented in Section III.3 after the flavon fields acquire their vacuum expectation values. Usually, the vacuum expectation values of fields are smaller than the scale of new physics which suppresses terms with higher mass dimension in the Kähler potential. Hence, the extra contributions to $\hat{\mathcal{K}}$ can be meaningfully split off to write

$$\hat{\mathcal{K}}^{ij} = \delta^{ij} + \Delta\hat{\mathcal{K}}^{ij} \tag{1.11}$$

with entries in $\Delta\hat{\mathcal{K}}$ smaller than one. The determination of $\Delta\hat{\mathcal{K}}$ and an analytical estimation of its effects on neutrino mixing are the topic of the following analysis.

From equation (1.5) and equation (1.10) it is clear that the discussion is not limited to supersymmetric theories. One can, and in an effective theory should, add interaction terms of the form (1.5) to any Lagrangian irrespective of whether it is supersymmetric or not. After plugging in the vacuum expectation values, one ends up with re-normalised kinetic terms like (1.10). The discussion could hence be led by starting with a non-supersymmetric Lagrangian with interactions that affect the kinetic terms encoded in a field-dependent matrix $\mathcal{K}$ such that

$$\mathcal{L} \supset \mathcal{K}^{ij}(\varphi, \varphi^*)\left(\frac{\mathrm{i}}{2}\,\psi_i^\dagger\,\bar{\sigma}^\mu\,\partial_\mu\psi_j - \frac{\mathrm{i}}{2}\,(\partial_\mu\psi_i^\dagger)\,\bar{\sigma}^\mu\,\psi_j\right) \xrightarrow{\varphi\to\langle\varphi\rangle} \hat{\mathcal{K}}^{ij}\,\mathrm{i}\,\psi_i^\dagger\,\bar{\sigma}^\mu\,\partial_\mu\psi_j \tag{1.12}$$

with $\hat{\mathcal{K}} \neq \mathbb{1}$. Thus, although the notation and terminology used here stems from supersymmetry, most of the results are also applicable to non-supersymmetric models. In fact, this is used in Section V.4.2, where the discussion is applied to a non-supersymmetric T′ model. For simplicity, $\hat{\mathcal{K}}$ is also called Kähler metric in the non-supersymmetric case.

V.2 Kähler corrections to lepton flavour mixing

The normalisation changes due to Kähler potential interactions have important implications for neutrino flavour mixing, cf. [130, 131]. Since these effects are to be quantified below, it is instructive to have a realistic example model at hand from the beginning. For this, the neutrino model of Section III.3 is used in its supersymmetric version. That is, all matter, Higgs and flavon fields of Table III.5 are elevated to chiral superfields. The Kähler potential just contains the canonical term for each field and the mass terms are now part of the superpotential,

$$\begin{aligned} W_m = {} & \frac{h_e}{\Lambda}\,H_d\,E^c\,(\Phi_e \otimes L)_{\mathbf{1}} + \frac{h_\mu}{\Lambda}\,H_d\,M^c\,(\Phi_e \otimes L)_{\mathbf{1}'} + \frac{h_\tau}{\Lambda}\,H_d\,T^c\,(\Phi_e \otimes L)_{\mathbf{1}''} \\ & + \frac{\lambda_1}{\Lambda\Lambda_\nu}\left\{\left[(L\,H_u) \otimes (L\,H_u)\right]_{\mathbf{3}_\mathrm{s}} \otimes \Phi_\nu\right\} + \frac{\lambda_2}{\Lambda\Lambda_\nu}\left[(L\,H_u) \otimes (L\,H_u)\right]_{\mathbf{1}}\,\Xi\,, \end{aligned} \tag{2.1}$$

where the superfields are denoted by the capitalised versions of the symbols introduced in Table III.5. The lower case symbols retain their old meaning, i.e. they denote the spinor components of matter fields and the scalar components of Higgs and flavon fields such that their notation coincides with the non-supersymmetric case.

The results for neutrino masses and the mixing parameters are identical to the ones presented earlier for the non-supersymmetric case. Thus, the effective mass matrices

$$W_m \xrightarrow{\varphi\to\langle\varphi\rangle} \frac{1}{2} L^T m_\nu L - R^T m_e L\,, \qquad R^T := (E^c, M^c, T^c)\,, \tag{2.2}$$

are again given by (III.3.2); hence, the model predicts tri-bi-maximal mixing while being able to accommodate the present knowledge of neutrino and charged lepton masses. These model predictions are perturbed by higher-order terms in the superpotential and by associated changes in the vacuum alignment, cf. [10]. Since the purpose of the present analysis is only the discussion of Kähler potential corrections, no such higher-order terms are added to the superpotential.

The prediction of tri-bi-maximal mixing rests on the assumption that the Kähler potential for the lepton fields is canonical,

$$K \supset L^\dagger L + R^\dagger R\,. \tag{2.3}$$

It is simple, however, to write down additional Kähler potential terms allowed by all symmetries such that

$$K \supset L^\dagger \mathcal{K}_L L + R^\dagger \mathcal{K}_R R = L^\dagger \left(\mathbb{1} + \Delta\mathcal{K}_L\right) L + R^\dagger \left(\mathbb{1} + \Delta\mathcal{K}_R\right) R \tag{2.4}$$

with non-trivial $\Delta\mathcal{K}_{L/R}$, which depend on the flavon fields Φ_e, Φ_ν and Ξ. The terms

$$\Delta K = \sum_{i\in\{\mathrm{a},\,\mathrm{s}\}} \left(\frac{\kappa_\nu^i}{\Lambda} L^\dagger (L \otimes \Phi_\nu)_{\mathbf{3}_i} + \frac{\kappa_e^i}{\Lambda} L^\dagger (L \otimes \Phi_e)_{\mathbf{3}_i} \right) + \frac{\kappa_\Xi}{\Lambda} \Xi L^\dagger L + \mathrm{h.\,c.}\,, \tag{2.5}$$

linear in the flavons might serve as an example. The discussion of these specific terms is deferred to Section V.4.1

In the low-energy theory, i.e. below the flavour symmetry breaking scale, the kinetic terms of the leptons are then

$$L^\dagger \hat{\mathcal{K}}_L L + R^\dagger \hat{\mathcal{K}}_R R = L^\dagger \left(\mathbb{1} + \Delta\hat{\mathcal{K}}_L\right) L + R^\dagger \left(\mathbb{1} + \Delta\hat{\mathcal{K}}_R\right) R \tag{2.6}$$

with, by construction, Hermitian matrices $\hat{\mathcal{K}}_{L/R}$. This necessitates a re-definition of the lepton fields L and R in order to arrive at canonically normalised fields L' and R' for which the mixing parameters and masses can then be read off from the superpotential. Since fields should not acquire a negative kinetic energy, the matrices $\hat{\mathcal{K}}_{L/R}$ can be assumed to be positive.[3] Hence, they have unique positive, Hermitian square roots $\hat{\mathcal{K}}_{L/R}^{1/2}$, see Section A.6.1, and one can write the kinetic terms as

$$L^\dagger \hat{\mathcal{K}}_L L + R^\dagger \hat{\mathcal{K}}_R R = L^\dagger \left(\hat{\mathcal{K}}_L^{1/2}\right)^\dagger \hat{\mathcal{K}}_L^{1/2} L + R^\dagger \left(\hat{\mathcal{K}}_R^{1/2}\right)^\dagger \hat{\mathcal{K}}_R^{1/2} R =: (L')^\dagger L' + (R')^\dagger R'\,. \tag{2.7}$$

3 In fact, if the corrections $\Delta\hat{\mathcal{K}}_{L/R}$ are large enough to drive any of the eigenvalues of $\hat{\mathcal{K}}_{L/R}$ to negative values, the effective theory description in general and the separation (1.11) in particular are not meaningful.

It is important to note that the field re-definitions

$$L' := \hat{\mathcal{K}}_L^{1/2}\, L\,, \tag{2.8a}$$
$$R' := \hat{\mathcal{K}}_R^{1/2}\, R \tag{2.8b}$$

are, in general, not unitary. This reflects the possibility that the normalisation of fields is changed.

The re-definition affects the mass terms in the superpotential in such a way that

$$\begin{aligned} W_m \xrightarrow{\varphi\to\langle\varphi\rangle} \frac{1}{2}\,(L')^T\,(\hat{\mathcal{K}}_L^{-1/2})^T\, m_\nu\, \hat{\mathcal{K}}_L^{-1/2}\, L' - (R')^T\,(\hat{\mathcal{K}}_R^{-1/2})^T\, m_e\, \hat{\mathcal{K}}_L^{-1/2}\, L' \\ =: \frac{1}{2}\,(L')^T\, m'_\nu\, L' - (R')^T\, m'_e\, L'\,, \end{aligned} \tag{2.9}$$

where mass matrices m'_ν and m'_e for the new fields are defined [130, 131]. It is these matrices that the mixing angles should be read off from and not the naive, i.e. unperturbed, matrices m_ν and m_e. The true mixing angles and phases can therefore be expected to be different from the naive expectations. This change of the mixing parameters from the naive to the true values is directly quantified by the analytical formulas derived in the following section. The reader not interested in the details of the derivation can skip to the results and examples presented in Section V.4.

V.3 Derivation of analytical formulas

The situation envisaged in the present section is that one is given a model with predictions for the mixing matrix U_{PMNS} computed assuming a canonical Kähler potential.[4] The purpose of the following derivation is to obtain formulas that give an estimate directly of the changes of the mixing parameters, i.e. without first computing the new mass matrices m'_ν and m'_e. This is also reflected by the fact that the input is only the naive mixing matrix U_{PMNS} and not the original mass matrices. The formulas are, therefore, completely agnostic about the details of the model. A model-dependence is only introduced when discussing which terms can enter the Kähler potential, a question whose answer depends on the symmetries, field content and VEV alignment of the model. This is discussed after the derivation of the general formulas in Section V.4. Note again that the discussion, although for simplicity phrased in supersymmetric terminology, also applies to the non-supersymmetric case.

The derivation of the analytical formulas depends on the assumption that the additional terms in the Kähler potential are corrections to the canonical Kähler potential, i.e. that they lead to small deviations from the unit matrix for the Kähler metric. This is a reasonable assumption because any higher-order term is suppressed by the ratio of a flavon VEV to the new physics scale, which is usually roughly equal to or lower than 0.2 in flavour models.[5] The true Kähler metrics for left-handed and right-handed lepton fields are parametrised as[6]

$$\hat{\mathcal{K}}_{L/R} =: \mathbb{1} - 2\, x_{L/R}\, P_{L/R}\,, \tag{3.1}$$

4 Whether higher-order terms in the superpotential have been taken into account is irrelevant for the discussion. However, it is, of course, advisable to do so.

5 This number is of the order of the Cabibbo angle, which, in quark flavour models, sets the scale of VEVs necessary to obtain a viable CKM matrix.

6 Note that this normalisation is only adopted for the derivation. As detailed below in Section V.3.3, the final formulas implemented in the package are computed for the simpler normalisation $\hat{\mathcal{K}}_{L/R} =: \mathbb{1} + x_{L/R}\, P_{L/R}$.

where $P_{L/R}$ are matrices later to be determined from the model with order one entries and where factors of two are introduced for later convenience. The assumption of small corrections thus implies that the real numbers $x_{L/R}$, which contain factors of VEV over scale, are small and can be used as expansion parameters. The field re-definition (2.8) can then be reversed using first the linear approximation

$$\hat{\mathcal{K}}_{L/R}^{1/2} \doteq \mathbb{1} - x_{L/R}\, P_{L/R} \tag{3.2}$$

for the square root and then the Neumann series [139] for the inverse truncated at linear order in $x_{L/R}$,

$$L \doteq (\mathbb{1} + x_L\, P_L)\; L' \,, \tag{3.3a}$$
$$R \doteq (\mathbb{1} + x_R\, P_R)\; R' \,. \tag{3.3b}$$

Using these approximate field re-definitions, one obtains approximations to the true mass matrices defined in (2.9) to first order in $x_{L/R}$ from the naive mass matrices by

$$m'_\nu = \left(\hat{\mathcal{K}}_L^{-1/2}\right)^T m_\nu\, \hat{\mathcal{K}}_L^{-1/2} \doteq m_\nu + x_L\, \left(P_L^T\, m_\nu + m_\nu\, P_L\right) \,, \tag{3.4a}$$
$$m'_e = \left(\hat{\mathcal{K}}_R^{-1/2}\right)^T m_e\, \hat{\mathcal{K}}_L^{-1/2} \doteq m_e + x_R\, P_R^T\, m_e + x_L m_e\, P_L \,. \tag{3.4b}$$

For the duration of the derivation, the true mass matrices are considered functions of $x_{L/R}$. They have to be diagonalised by a Takagi factorisation and a singular value decomposition,[7] respectively,

$$m'_\nu(x_L) = U_\nu^*(x_L)\, D_\nu(x_L)\, U_\nu^\dagger(x_L) \,, \tag{3.5a}$$
$$m'_e(x_L, x_R) = V_e(x_L, x_R)\, D_e(x_L, x_R)\, U_e^\dagger(x_L, x_R) \,, \tag{3.5b}$$

where $D_{\nu/e}$ are diagonal matrices with non-negative real entries, i.e. they contain the singular values (masses) of m'_ν and m'_e. Since the latter are functions of $x_{L/R}$, the singular values and the diagonalising matrices are also functions of these variables. This immediately carries over to the PMNS matrix

$$U_{\text{PMNS}}(x_L, x_R) = U_e^\dagger(x_L, x_R)\, U_\nu(x_L) \,. \tag{3.6}$$

The basic idea is to think of $U_{\text{PMNS}}(x_L, x_R)$ as being determined by an initial value problem with $U_{\text{PMNS}}(0,0)$ being the original PMNS matrix before taking into account the Kähler corrections. The corresponding differential equations can be read off from (3.4). Since they are structurally identical to the renormalisation group equations for the neutrino mixing parameters, they can be treated in the same fashion [94].

For computational reasons it is advantageous to introduce for each unitary matrix U depending on a variable x an associated anti-Hermitian matrix

$$T := U^\dagger\, \dot{U} \,, \tag{3.7}$$

where $\dot{U}$ is the derivative of U with respect to x. It will always be clear from the context or specified explicitly which variable the derivative refers to. This matrix allows to write the

7 See again Section III.1, Section A.6.3 and Section A.6.2.

derivative of U as $\dot{U} = UT$. As an anti-Hermitian 3×3 matrix, T has nine real degrees of freedom

$$\operatorname{Re} T_{i<j},\ \operatorname{Im} T_{i\leq j}\,, \qquad i,j = 1,2,3\,. \tag{3.8}$$

From its definition it is clear that the matrix T_{PMNS} depends linearly on the derivatives of all nine mixing parameters. Therefore, there is a linear map from the derivatives of the mixing parameters to the independent elements of T_{PMNS}, which can be inverted to obtain the desired linear map from the nine elements of T_{PMNS} to the nine derivatives of the mixing parameters. This computation has to be performed only once,[8] and the result is implemented in the MATHEMATICA package `KaehlerCorrections` presented in Section V.3.3.

The remaining task is to determine the dependence of the entries of T_{PMNS} on the matrices $P_{L/R}$. There are contributions coming from U_ν and U_e, respectively, which can be discussed separately. To this end, write

$$\begin{aligned} T_{\text{PMNS}} &= U_{\text{PMNS}}^\dagger\, \dot{U}_e^\dagger\, U_\nu + U_{\text{PMNS}}^\dagger\, U_e^\dagger\, \dot{U}_\nu \\ &= U_{\text{PMNS}}^\dagger\, \dot{U}_e^\dagger\, (U_e\, U_e^\dagger)\, U_\nu + U_{\text{PMNS}}^\dagger\, U_e^\dagger\, (U_\nu\, U_\nu^\dagger)\, \dot{U}_\nu \\ &= T_\nu - U_{\text{PMNS}}^\dagger\, T_e\, U_{\text{PMNS}}\,. \end{aligned} \tag{3.9}$$

In the first line the product rule was used, in the second line two identity matrices were inserted and in the last line the matrices T_e and T_ν were introduced and their anti-Hermiticity used.

Some more comments on the following computation are in order before proceeding. Only contributions linear in $x_{L/R}$ are taken into account. Moreover, the computation is assumed to proceed in a basis where m_e, i.e. the original neutrino mass matrix, is diagonal with real, non-negative entries. At the same time, it is assumed that the charged lepton phases $\delta_{e/\mu/\tau}$ are zero. Of course, after transforming to a basis with a diagonal charged lepton mass matrix with non-negative entries, there is no guarantee that these phases are zero. Indeed, this second assumption is not even fulfilled by the example model from Section III.3. Further, if the Kähler metric is not canonical, it is not invariant under the phase re-definitions needed to obtain zero charged lepton phases. Hence, in all such cases, one has to replace the matrices $P_{L/R}$ determined from the Kähler potential with

$$\hat{P}_{L/R} \coloneqq (U_e^{ph})^\dagger\, P_{L/R}\, U_e^{ph} \tag{3.10}$$

before using the formulas, where U_e^{ph} is the diagonal phase matrix used to remove the phases from U_{PMNS}, see Section III.1.

Since the computations relating $P_{L/R}$ with T_e and T_ν differ, the discussion is now split into two parts. The neutrino contribution is treated first.

V.3.1 Corrections to m_ν

The true neutrino mass matrix (3.4a) is, to linear order in x_L, a solution to the initial value problem

$$\frac{\mathrm{d}}{\mathrm{d}x_L}\, m_\nu'(x_L) = P_L^T\, m_\nu + m_\nu\, P_L\,, \qquad m_\nu'(0) = m_\nu\,. \tag{3.11}$$

8 To be precise, it has to be done once for any given parametrisation of the mixing matrix U_{PMNS}. The package implements the map for the standard parametrisation (III.1.7).

Plugging in the Takagi factorisation of the neutrino mass matrix and evaluating the expression at $x_L = 0$, one arrives at

$$\frac{\mathrm{d}}{\mathrm{d}x_L}\left(U_\nu^*(x_L)\, D_\nu(x_L)\, U_\nu^\dagger(x_L)\right)\Big|_{x_L=0} = P_L^T\, U_\nu^*(0)\, D_\nu(0)\, U_\nu^\dagger(0) + U_\nu^*(0)\, D_\nu(0)\, U_\nu^\dagger(0)\, P_L\,. \tag{3.12}$$

The argument 0 is understood and suppressed henceforth. Moreover, define the abbreviation

$$\tilde{P}_L \coloneqq U_\nu^\dagger\, P_L\, U_\nu = U_{\mathrm{PMNS}}^\dagger\, P_L\, U_{\mathrm{PMNS}}\,, \tag{3.13}$$

where the latter equality is correct because $U_e(0,0)$ is, by the basis choice, the identity matrix. Using the product rule and multiplying the equation with U_ν^T from the left and U_ν from the right, one obtains

$$U_\nu^T\, \dot{U}_\nu^*\, D_\nu + D_\nu\, \dot{U}_\nu^\dagger\, U_\nu + \dot{D}_\nu = \tilde{P}_L^T\, D_\nu + D_\nu\, \tilde{P}_L\,. \tag{3.14}$$

Introducing the anti-Hermitian matrix T_ν as explained before, one can rewrite this equation in the more useful form

$$\dot{D}_\nu = \tilde{P}_L^T\, D_\nu + D_\nu\, \tilde{P}_L - T_\nu^*\, D_\nu + D_\nu\, T_\nu\,. \tag{3.15}$$

By definition, the matrix D_ν is real and diagonal; hence, this must also be true for the right-hand side. Consider first the equations for the diagonal entries, where the diagonal entries of D_ν are the neutrino masses denoted by m_{ν_i} (no sum over i):

$$\dot{m}_{\nu_i} = 2\,(\tilde{P}_L)_{ii}\, m_{\nu_i} + \left((T_\nu)_{ii} - (T_\nu^*)_{ii}\right)\, m_{\nu_i}\,. \tag{3.16}$$

Whereas P_L and thus $\tilde{P}_L$ is Hermitian and has real diagonal values, the imaginary parts of the diagonal of T_ν must vanish,

$$\mathrm{Im}\,(T_\nu)_{ii} = 0\,, \tag{3.17}$$

for this equation to be consistent. The equation of the (i,j) position is

$$m_{\nu_i}\,(T_\nu)_{ij} + (T_\nu^*)_{ij}\, m_{\nu_j} = -(\tilde{P}_L^T)_{ij}\, m_{\nu_j} - m_{\nu_i}\,(\tilde{P}_L)_{ij}\,. \tag{3.18}$$

This set of equations can then be solved for the real and imaginary parts of T_ν in terms of the $\tilde{P}_L$:

$$\mathrm{Re}(T_\nu)_{ij} = -\frac{m_{\nu_i} + m_{\nu_j}}{m_{\nu_i} - m_{\nu_j}}\, \mathrm{Re}(\tilde{P}_L)_{ij}\,, \qquad i \neq j\,, \tag{3.19a}$$

$$\mathrm{Im}(T_\nu)_{ij} = -\frac{m_{\nu_i} - m_{\nu_j}}{m_{\nu_i} + m_{\nu_j}}\, \mathrm{Im}(\tilde{P}_L)_{ij}\,. \tag{3.19b}$$

This fully specifies T_ν in terms of P_L and the original U_{PMNS}.

V.3.2 Corrections to m_e

In complete analogy to the corrections to the neutrino diagonalisation matrix U_ν, one can also compute the corrections to U_e. The true charged lepton mass matrix (3.4b) can be diagonalised by the singular value decomposition (3.5b). However, for the PMNS matrix, only U_e is needed such that it is more convenient to consider

$$m'_e(x_L, x_R)^\dagger \, m'_e(x_L, x_R) = U_e(x_L, x_R) \, D_e^2(x_L, x_R) \, U_e^\dagger(x_L, x_R) \,, \tag{3.20}$$

which to first order in $x_{L/R}$ is

$$m_e^2 + 2\, x_R \, m_e \, P_R^T \, m_e + x_L \, \left(P_L \, m_e^2 + m_e^2 \, P_L\right) = U_e(x_L, x_R) \, D_e^2(x_L, x_R) \, U_e^\dagger(x_L, x_R) \,, \tag{3.21}$$

where it has been used that m_e is diagonal in the chosen basis. The contributions connected to x_L and x_R are discussed in turn.

First, take the derivative of (3.21) with respect to x_L and evaluate the expression at $x_L = x_R = 0$, suppressing the dependence on x_R:

$$\frac{\mathrm{d}}{\mathrm{d}x_L} \left(U_e(x_L) \, D_e^2(x_L) \, U_e^\dagger(x_L)\right)\Big|_{x_{L/R}=0} = P_L \, m_e^2 + m_e^2 \, P_L \,. \tag{3.22}$$

Using the product rule and introducing $T_e^L = \dot{U}_e$, where the superscript L means that the derivative is taken with respect to x_L and where $U_e(0) = \mathbb{1}$ is used, this equation can be rewritten to (the argument 0 is again suppressed)

$$\dot{D}_e^2 = P_L \, m_e^2 + m_e^2 \, P_L - T_e^L \, m_e^2 + m_e^2 \, T_e^L \,. \tag{3.23}$$

Let the charged lepton masses be denoted by m_{e_i}. Then the equations determining the diagonal values are

$$\dot{m}_{e_i}^2 = 2 \, (P_L)_{ii} \, m_{e_i}^2 \,. \tag{3.24}$$

Note that the contribution from T_e^L drops completely out of the equation; thus, the diagonal values of T_e^L cannot be determined. This reflects the fact that after diagonalising the Kähler potential the charged lepton phases can again be changed arbitrarily. During the computation of the formulas for the MATHEMATICA package, the diagonal entries of T_e^L were kept arbitrary such that it could be verified explicitly that they drop out of the formulas for all physical mixing parameters, i.e. for angles, δ_{CP} and the Majorana phases. The off-diagonal values of T_e^L, however, can be computed from the equations above and are

$$\left(T_e^L\right)_{ij} = -\frac{m_{e_i}^2 + m_{e_j}^2}{m_{e_i}^2 - m_{e_j}^2} \, (P_L)_{ij} \,, \qquad i \neq j \,. \tag{3.25}$$

It remains to determine T_e^R, which encodes the contribution connected to x_R. The analogue of (3.23) is

$$\dot{D}_e^2 = 2 \, m_e \, P_R^T m_e - T_e^R \, m_e^2 + m_e^2 \, T_e^R \,. \tag{3.26}$$

Again, the diagonal entries of T_e^R are not determined but only affect the charged lepton phases, which can be rotated away in the end. This has also been explicitly verified. The off-diagonal terms are

$$\left(T_e^R\right)_{ij} = -2 \, \frac{m_{e_i} \, m_{e_j}}{m_{e_i}^2 - m_{e_j}^2} \, (P_R)_{ji} \,, \qquad i \neq j \,. \tag{3.27}$$

This finishes the computation of the matrices T_i in terms of $P_{L/R}$. Examples for the corrections to be expected are presented in Section V.4.

V.3.3 The package `KaehlerCorrections`

The formulas derived by the procedure described above are implemented in the package `KaehlerCorrections` for MATHEMATICA [11]. It can be found on the web-page

http://einrichtungen.ph.tum.de/T30e/codes/KaehlerCorrections.

The package contains the full analytical formulas for left- and right-handed corrections due to a Kähler potential of the form

$$K = L^\dagger\,(\mathbb{1} + x_L\,P_L)\,L + R^\dagger\,(\mathbb{1} + x_R\,P_R)\,R \tag{3.28}$$

or due to the corresponding kinetic terms in the non-supersymmetric case. Note the different normalisation of $x_{L/R}$ compared to (3.1).

The initial values, i.e. the mixing parameters and masses for the theory with canonical Kähler potential, $x_L = x_R = 0$, can be set by the user. This can most easily be done using the function `kaehlerCorr`. An example for how this function can be called looks as follows:

$$\begin{array}{ccccccc} & & 0 & & & & \{m_{\nu_1}, m_{\nu_2}, m_{\nu_3}, m_e, m_\mu, m_\tau\} \\ & & \downarrow & & & & \downarrow \\ \text{kaehlerCorr}[& P_L, & P_R, & \text{initial angles \& phases}, & & \text{initial masses} &] \\ & \uparrow & & \uparrow & & & \\ & \begin{pmatrix} 0 & \mathrm{i} & -\mathrm{i} \\ -\mathrm{i} & 0 & \mathrm{i} \\ \mathrm{i} & -\mathrm{i} & 0 \end{pmatrix} & & \left\{\arcsin\left(\frac{1}{\sqrt{3}}\right), 0, \frac{\pi}{4}, \delta_0, \pi, \pi, 0, 2\pi, 2\pi\right\} & & \end{array}$$

The formulas are computed for a diagonal charged lepton mass matrix with non-negative real entries. If the charged lepton mass matrix of the model at hand does not fulfil the requirement, one has to transform to such a basis before using the package to compute the corrections.

If one of the mixing angles initially is zero, as happens with tri-bi-maximal mixing, the phase δ_{CP} is not well defined. Its correct value can be obtained by demanding that the change of δ_{CP} be analytical in the angle that has zero initial value, see also the discussion in Section V.4.1. This computation is performed automatically by the package. However, there also is the possibility to override this behaviour in case the automatic determination fails.

More information on the package can be found in the manual which is part of the download.

V.4 Results and examples

Before discussing explicit examples, let us summarise the findings of the derivation. There is a linear relation between the matrix T_{PMNS} defined in (3.9) and the first derivatives of the mixing angles with respect to $x_{L/R}$. The contributions of charged leptons and neutrinos and of left-handed doublets and right-handed singlets can be discussed separately, writing

$$T^L_{\text{PMNS}} = T_\nu - U^\dagger_{\text{PMNS}}\,T^L_e\,U_{\text{PMNS}}\,, \tag{4.1a}$$
$$T^R_{\text{PMNS}} = -U^\dagger_{\text{PMNS}}\,T^R_e\,U_{\text{PMNS}}\,. \tag{4.1b}$$

The entries of T_{PMNS} are, to first order in $x_{L/R}$, determined by

$$\text{Re}(T_\nu)_{ij} = -\frac{m_{\nu_i} + m_{\nu_j}}{m_{\nu_i} - m_{\nu_j}}\,\text{Re}(U^\dagger_{\text{PMNS}}\,P_L\,U_{\text{PMNS}})_{ij}\,, \qquad i \neq j\,, \tag{4.2a}$$

$$\mathrm{Im}(T_\nu)_{ij} = -\frac{m_{\nu_i} - m_{\nu_j}}{m_{\nu_i} + m_{\nu_j}} \,\mathrm{Im}(U^\dagger_{\mathrm{PMNS}}\, P_L\, U_{\mathrm{PMNS}})_{ij}\,, \tag{4.2b}$$

$$\left(T_e^L\right)_{ij} = -\frac{m_{e_i}^2 + m_{e_j}^2}{m_{e_i}^2 - m_{e_j}^2}\,(P_L)_{ij}\,, \qquad i \neq j\,, \tag{4.2c}$$

$$\left(T_e^R\right)_{ij} = -2\,\frac{m_{e_i}\, m_{e_j}}{m_{e_i}^2 - m_{e_j}^2}\,(P_R)_{ji}\,, \qquad i \neq j \tag{4.2d}$$

in terms of $P_{L/R}$. The missing imaginary parts of the diagonals of $T_e^{L/R}$ are undetermined but only influence the change of the charged lepton phases, which, in the low-energy theory, are unphysical. The formulas thus yield a linear approximation to the effects induced by additional terms in the Kähler potential changing the Kähler metric by $-2\,x_{L/R}\,P_{L/R}$. For completely general initial conditions, the formulas are rather complicated and can be found in the MATHEMATICA package `KaehlerCorrections`. However, for symmetric starting points like tri-bi-maximal mixing, the formulas are rather simple as is shown for some examples explicitly below and in Appendix B.

From the formulas (4.2) it is obvious that the mass spectrum plays a crucial role for the size of the corrections. In particular, the effects depend on the mass differences of the neutrinos and the differences of the mass squares of the charged leptons. Since the charged lepton masses are highly hierarchical, $m_e \ll m_\mu \ll m_\tau$, T_e^L is, up to signs, almost the same as P_L whereas T_e^R is highly suppressed. Indeed, to first order in the mass differences, T_e^R has entries proportional to $m_e/m_\mu \approx 1/200$, $m_e/m_\tau \approx 1/3500$ and $m_\mu/m_\tau \approx 1/17$ and is therefore practically negligible. The contributions coming from the neutrinos are certainly not negligible, as shown below, and become more important if their masses are degenerate. This resembles the results for the renormalisation group effects [94]. However, in contrast to these effects, the Kähler corrections are not suppressed by a loop factor. Moreover, the Kähler corrections are not restricted to diagonal matrices $P_{L/R}$ as can be seen from the examples presented below. In particular, there is no reason to assume that the largest entries of $P_{L/R}$ are in the lower-right corner as is the case for the renormalisation group effects which are dominated by the tau lepton Yukawa coupling y_τ.

Let us now discuss the structure of additional Kähler potential terms and quantify their implications. The first example discussed is the A_4 model already introduced above. As a second example, an extension of this model using T′ is used, and, finally, some general formulas and results are presented.

V.4.1 Kähler corrections to the A_4 model

Let us start the discussion of Kähler corrections to the A_4 model of Section V.2 with the right-handed charged lepton corrections. Even ignoring their large suppression by the mass splittings, the model is such that one cannot expect any effects on the mixing angles. The reason is that the charged lepton singlets are in one-dimensional irreducible representations of A_4, whereas there are no flavons in non-trivial one-dimensional representations. Thus, one cannot generate off-diagonal terms for the Kähler metric and only the mass eigenvalues are changed by canonical normalisation. Hence, only additional Kähler potential terms for the left-handed doublets are considered here.

The simplest terms one can write down that are compatible with gauge and A_4 symmetries are linear in the flavons. They are expected to give the largest contributions because they are only suppressed by one power of VEV divided by new physics scale in the effective field

theory expansion. These linear terms in the flavon fields contributing to the Kähler metric $\Delta\mathcal{K}_L$ of the left-handed fields for the A_4 model are

$$\Delta K = \sum_{i\in\{a,\,s\}} \left(\frac{\kappa_\nu^i}{\Lambda} L^\dagger \left(L \otimes \Phi_\nu\right)_{\mathbf{3}_i} + \frac{\kappa_e^i}{\Lambda} L^\dagger \left(L \otimes \Phi_e\right)_{\mathbf{3}_i} \right) + \frac{\kappa_\Xi}{\Lambda}\, \Xi\, L^\dagger L + \text{h. c.} \tag{4.3}$$

The last term is a multiple of the canonical Kähler potential for the lepton doublets and only changes the mass eigenvalues. It is thus not considered in the following. Spelt out explicitly, the A_4 contractions of the other terms are

$$\begin{aligned} L^\dagger \left(L \otimes \Phi\right)_{\mathbf{3}_s} = \frac{1}{\sqrt{6}} \big[& L_1^\dagger \left(2 L_1 \Phi_1 - L_2 \Phi_3 - L_3 \Phi_2\right) + L_2^\dagger \left(2 L_3 \Phi_3 - L_1 \Phi_2 - L_2 \Phi_1\right) \\ & + L_3^\dagger \left(2 L_2 \Phi_2 - L_1 \Phi_3 - L_3 \Phi_1\right) \big] , \end{aligned} \tag{4.4a}$$

$$\begin{aligned} L^\dagger \left(L \otimes \Phi\right)_{\mathbf{3}_a} = \frac{1}{\sqrt{2}} \big[& L_1^\dagger \left(L_2 \Phi_3 - L_3 \Phi_2\right) + L_2^\dagger \left(L_1 \Phi_2 - L_2 \Phi_1\right) \\ & + L_3^\dagger \left(L_3 \Phi_1 - L_1 \Phi_3\right) \big] , \end{aligned} \tag{4.4b}$$

where Φ can be Φ_e or Φ_ν. Plugging in the VEVs one arrives at the additional contributions to the Kähler metric

$$\Delta\hat{\mathcal{K}}_L = \kappa_e^s \frac{v'}{\Lambda} \frac{1}{\sqrt{6}} P_e^s + \kappa_e^a \frac{v'}{\Lambda} \frac{1}{\sqrt{2}} P_e^a + \kappa_\nu^s \frac{v}{\Lambda} \frac{1}{\sqrt{6}} P_\nu^s + \kappa_\nu^a \frac{v}{\Lambda} \frac{1}{\sqrt{2}} P_\nu^a + \text{h. c.} , \tag{4.5}$$

where the following abbreviations for matrices are introduced:

$$P_e^s := \text{diag}\left(2, -1, -1\right) , \tag{4.6a}$$

$$P_e^a := \text{diag}\left(0, -1, 1\right) , \tag{4.6b}$$

$$P_\nu^s := \begin{pmatrix} 2 & -1 & -1 \\ -1 & -1 & 2 \\ -1 & 2 & -1 \end{pmatrix} , \tag{4.6c}$$

$$P_\nu^a := \begin{pmatrix} 0 & 1 & -1 \\ 1 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix} . \tag{4.6d}$$

In fact, not all of these terms are allowed in the model. The neutrino flavon triplet Φ_ν is additionally charged under the $\mathbb{Z}_4$ shaping symmetry, see Table III.5, such that $\kappa_\nu^{a/s}$ vanish. This highlights a general feature of Kähler potential terms linear in the flavons: they can easily be forbidden by additional abelian shaping symmetries. In certain models, there are enough such symmetries present from the outset in order to get rid of all linear terms, see e.g. the T′ model discussed below in Section V.4.2. Hence, although if present they should have the largest effects, linear terms are not further discussed here.

In contrast to linear terms, terms quadratic in a particular flavon cannot be forbidden by abelian symmetries. That is, terms of the form

$$\left(L \otimes \Phi\right)_R^\dagger \left(L \otimes \Phi\right)_R \tag{4.7}$$

are always present. They can only be forbidden by enlarging the non-abelian flavour symmetry, in which case one would have to consider Kähler corrections to the model with the larger symmetry group. Thus, the problem would be transformed rather than solved.

The simplest example of such a quadratic correction is

$$\frac{1}{\Lambda^2}\,(L\otimes\Phi)^\dagger_{\mathbf{1}}\,(L\otimes\Phi)_{\mathbf{1}} = \frac{1}{\Lambda^2}\,\left|(L_1\,\Phi_1 + L_2\,\Phi_3 + L_3\,\Phi_2)\right|^2\,. \tag{4.8}$$

It leads to the additional contributions

$$\Delta\hat{\mathcal{K}}_L = \kappa_e^{\mathbf{1}}\,\frac{|v'|^2}{\Lambda^2}\,\frac{1}{3}\,\mathrm{diag}\,(1,\,0,\,0) + \kappa_\nu^{\mathbf{1}}\,\frac{|v|^2}{\Lambda^2}\,\frac{1}{3}\begin{pmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{pmatrix} + \mathrm{h.\,c.} \tag{4.9}$$

to the Kähler metric. As is common to all quadratic terms, they are suppressed quadratically by the ratio of flavon VEV to scale Λ, i.e. their size is smaller than that of the linear terms. However, as seen explicitly below, the effects of quadratically suppressed terms are not necessarily small and certainly not negligible, in contrast to earlier claims in the literature [134].

A less simplistic contraction leading to quadratic corrections is

$$\begin{aligned}\frac{1}{\Lambda^2}\,(L\otimes\Phi)^\dagger_{\mathbf{3}_\mathrm{s}}\,(L\otimes\Phi)_{\mathbf{3}_\mathrm{a}} = \frac{1}{\Lambda^2}\,\frac{1}{2\sqrt{3}}\,\big[&\left(2\,L_1^\dagger\,\Phi_1^\dagger - L_2^\dagger\,\Phi_3^\dagger - L_3^\dagger\,\Phi_2^\dagger\right)\,\left(L_2\,\Phi_3 - L_3\,\Phi_2\right)\\ &+ \left(2\,L_3^\dagger\,\Phi_3^\dagger - L_2^\dagger\,\Phi_1^\dagger - L_1^\dagger\,\Phi_2^\dagger\right)\,\left(L_1\,\Phi_2 - L_2\,\Phi_1\right)\\ &+ \left(2\,L_2^\dagger\,\Phi_2^\dagger - L_1^\dagger\,\Phi_3^\dagger - L_3^\dagger\,\Phi_1^\dagger\right)\,\left(L_3\,\Phi_1 - L_1\,\Phi_3\right)\big]\,.\end{aligned} \tag{4.10}$$

This contraction is present for both Φ_e and Φ_ν, leading to the two additional Kähler potential terms

$$\Delta K = \kappa_e^{\mathrm{as}}\,\frac{1}{\Lambda^2}\,(L\otimes\Phi_e)^\dagger_{\mathbf{3}_\mathrm{s}}\,(L\otimes\Phi_e)_{\mathbf{3}_\mathrm{a}} + \tilde{\kappa}_\nu^{\mathrm{as}}\,\frac{1}{\Lambda^2}\,(L\otimes\Phi_\nu)^\dagger_{\mathbf{3}_\mathrm{s}}\,(L\otimes\Phi_\nu)_{\mathbf{3}_\mathrm{a}} + \mathrm{h.\,c.}\,, \tag{4.11}$$

where both couplings are, as always, complex numbers. Plugging in the VEVs, the Kähler metric is amended by

$$\Delta\hat{\mathcal{K}}_L = \kappa_e^{\mathrm{as}}\,\frac{|v'|^2}{\Lambda^2}\,\frac{1}{2\sqrt{3}}\,\mathrm{diag}\,(0,\,1,\,-1) + \kappa_\nu^{\mathrm{as}}\,\frac{|v|^2}{\Lambda^2}\,\frac{\sqrt{3}}{2}\begin{pmatrix}0 & \mathrm{i} & -\mathrm{i}\\ -\mathrm{i} & 0 & \mathrm{i}\\ \mathrm{i} & -\mathrm{i} & 0\end{pmatrix} + \mathrm{h.\,c.}\,, \tag{4.12}$$

where κ_ν^{as} is the imaginary part of $\tilde{\kappa}_\nu^{\mathrm{as}}$. The corresponding imaginary unit has been absorbed into the P matrix to render it Hermitian, and the contribution proportional to the real part of $\tilde{\kappa}_\nu^{\mathrm{as}}$ drops out because the Kähler potential is real. The second term is particularly interesting. On the one hand, as shown below, this term leads to large corrections to the mixing angle θ_{13}. On the other hand, this contribution to the Kähler metric is not CP invariant, i.e. it could be forbidden by a CP symmetry. For the details of CP symmetries compatible with A_4, see Chapter VII. Here it suffices to say that the CP transformation turns out to be just the canonical one. This symmetry forces $\tilde{\kappa}_\nu^{\mathrm{as}}$ to be real such that κ_ν^{as} vanishes.

Without going into further details of the computations, all correction matrices that occur at quadratic order can be written as linear combinations of the following five basis matrices:

$$P_\mathrm{I} := \mathrm{diag}\,(1,\,0,\,0)\,, \tag{4.13a}$$

$$P_\mathrm{II} := \mathrm{diag}\,(0,\,1,\,0)\,, \tag{4.13b}$$

θ_{12}	θ_{13}	θ_{23}	δ_{CP}	δ_e	δ_μ	δ_τ	α_1	α_2
$\operatorname{atan}\frac{1}{\sqrt{2}}$	0	$\frac{\pi}{4}$	–	π	π	0	$2\,\pi$	$2\,\pi$

Table V.1: Values for the mixing parameters of the A_4 model before taking into account Kähler corrections. The model precisely exhibits tri-bi-maximal mixing.

$$P_{\text{III}} := \operatorname{diag}(0,\,0,\,1)\,, \tag{4.13c}$$

$$P_{\text{IV}} := \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \tag{4.13d}$$

$$P_{\text{V}} := \begin{pmatrix} 0 & \mathrm{i} & -\mathrm{i} \\ -\mathrm{i} & 0 & \mathrm{i} \\ \mathrm{i} & -\mathrm{i} & 0 \end{pmatrix}. \tag{4.13e}$$

In fact, the matrices $P_{\text{I–III}}$ arise from contractions of Φ_e whereas P_{IV} and P_{V} arise from Φ_ν-related Kähler potential terms. The list also shows clearly that there is no reason to assume that the emerging P matrices are diagonal (like the ones dictating renormalisation group effects) or that their dominant entry is in the lower-right corner, in contrast to earlier claims [132]. In fact, it turns out that the non-diagonal contributions are the most important ones for the model at hand. This is, of course, not very surprising as non-diagonal entries in the Kähler metric mix the kinetic terms of the three generations, which intuitively can be expected to induce large changes of the mixing angles.

After discussing the possible contributions of the flavon VEVs to the Kähler metric in the A_4 model, the effects on the mixing angles shall now be quantified using the approximative analytical formulas derived in the previous section. The results obtained with these formulas are compared to the results of an exact numerical diagonalisation of the Kähler metric. In this case, the mixing parameters are extracted from the corrected mass matrices using the `MixingParameterTools` package for MATHEMATICA [95]. The initial values for the mixing parameters are taken from the PMNS matrix of the A_4 model shown in equation (III.3.4) with the mass parameters assumed to be real. These values are also shown in Table V.1. Note that the value of δ_{CP} is undefined because $\theta_{13} = 0$.[9] For the analytical formulas, one still has to provide an initial value for the CP phase. The correct value is obtained by demanding that the residue of the change of δ_{CP} at $\theta_{13} = 0$ vanishes, i.e. that δ_{CP} is an analytic function in θ_{13} also at zero. The package `KaehlerCorrections` presented in Section V.3.3 takes care of this automatically.

Concerning the hierarchy of neutrino masses, normal ordering is chosen. For the plots, the mass of the lightest neutrino m_{ν_1} is kept as a free parameter while the other masses are set relatively to it using the experimental values for the mass square differences shown in Table III.3.

Since the main deviation of the tri-bi-maximal prediction from experiment is in θ_{13}, it seems desirable to quantify the possible corrections to this mixing parameter first. The most relevant contribution is the one of the matrix P_{V} shown in (4.12). Note that this contribution can be forbidden by a CP symmetry. Accordingly, the initial value of δ_{CP} obtained by the analyticity criterion stated above is $\delta_{CP} = \pm\pi/2$. The analytical formula for the change of θ_{13}

9 Indeed, δ_{CP} is undefined if any of the mixing angles is zero because there is no CP violation in two-particle mixing.

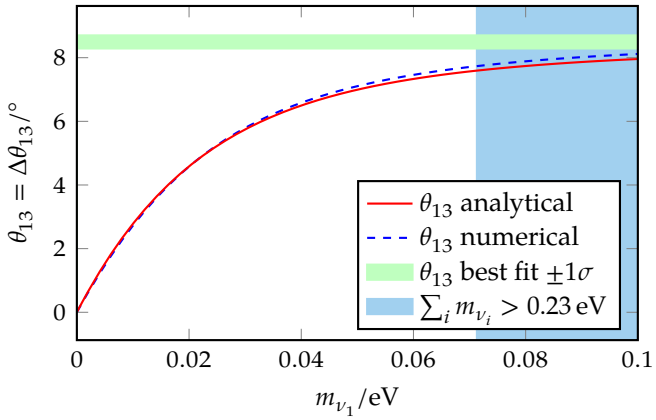


Figure V.1: Correction to θ_{13} in the A_4 model due to the additional Kähler metric contribution $\Delta\hat{\mathcal{K}}_L = \kappa_\nu^{\text{as}} \frac{|v|^2}{\Lambda^2} \sqrt{3}\, P_{\text{V}}$ in dependence of the lightest neutrino mass m_{ν_1}. The other neutrino masses are fixed by the measured mass differences. The free parameters are set to $|v|/\Lambda = 0.2$ and $\kappa_\nu^{\text{as}} = 3$ (see main text). The dashed blue line is an exact numerical computation and the solid red line shows the linear approximation discussed in the text. The green shaded area shows the $\pm 1\sigma$ range around the best fit point for θ_{13} and the blue shaded area the exclusion by the limit on the neutrino mass sum. Experimental values are taken from [40, 54].

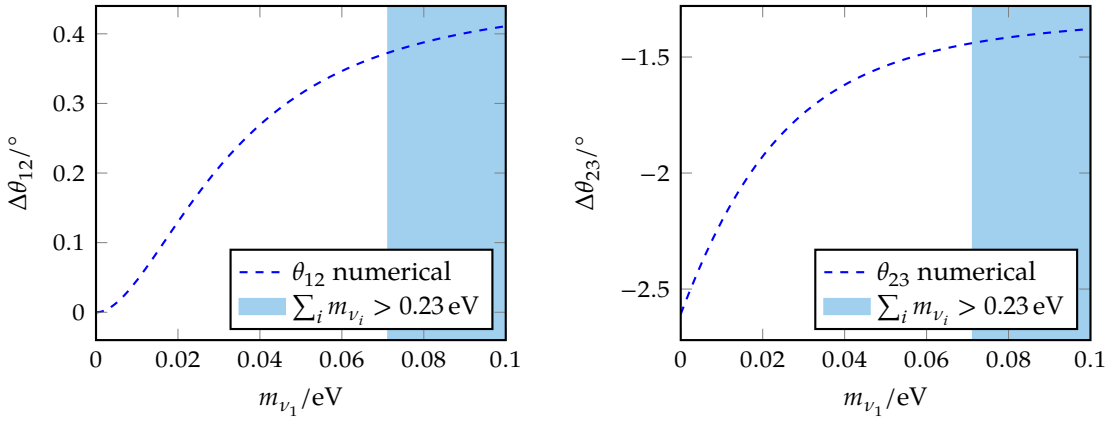
for the given initial condition of tri-bi-maximal mixing due to P_{V} is

$$\begin{aligned} \Delta\theta_{13} &= \kappa_e^{\text{as}} \frac{|v|^2}{\Lambda^2} \sqrt{\frac{3}{2}} \left(\frac{2\, m_{\nu_1}}{m_{\nu_1} + m_{\nu_3}} + \frac{m_e^2}{m_\mu^2 - m_e^2} + \frac{m_e^2}{m_\tau^2 - m_e^2} \right) \\ &\approx \kappa_e^{\text{as}} \frac{|v|^2}{\Lambda^2} \sqrt{6}\, \frac{m_{\nu_1}}{m_{\nu_1} + m_{\nu_3}}\,, \end{aligned} \tag{4.14}$$

where in the second line the contribution due to the charged leptons is dropped because of their mass hierarchy. The correction approaches a maximum for large values of the lightest neutrino mass m_{ν_1}, i.e. for a degenerate spectrum, as already predicted by the general considerations above.

In Figure V.1, the change of θ_{13} is plotted with respect to the mass m_{ν_1}. The parameters are chosen such that $|v|/\Lambda = 0.2$, i.e. the ratio of VEV to scale is of the order of the Cabibbo angle, and such that $\kappa_\nu^{\text{as}} = 3$. The reason for this seemingly very large coupling value is the normalisation of the Clebsch–Gordan coefficients, see Section II.6. The normalisation adopted here is such that the Clebsch–Gordan matrix is unitary, which means that the more terms there are in a contraction the smaller are the coefficients. However, a more physical condition is that the numbers multiplying specific monomials in the potential should not exceed order one. A value of precisely one would, in the present case, be achieved for a coupling of $2\sqrt{3}$, which cancels the normalisation factors of the Clebsch–Gordan coefficients. To facilitate the comparison with the original publication, this has been rounded down to 3 such that the numerical results coincide.[10] Note that, despite the large value of the coupling, the expansion parameter x_L is still only of order 0.1, i.e. any higher-order contributions neglected by the analytical formulas can be expected to be subleading. Indeed, there is a

10 There are small differences to the numerical results of the original publication because of the newer values for the mass-square differences used here.



(a) Correction to θ_{12}.

(b) Correction to θ_{23}.

Figure V.2: Corrections to (a) θ_{12} and (b) θ_{23} in the A_4 model due to the additional Kähler metric contribution $\Delta\hat{\mathcal{K}}_L = \kappa_\nu^{\mathrm{as}} \frac{|v|^2}{\Lambda^2} \sqrt{3}\, P_V$ in dependence of the lightest neutrino mass m_{ν_1}. The other neutrino masses are fixed by the measured mass differences. The free parameters are set to $|v|/\Lambda = 0.2$ and $\kappa_\nu^{\mathrm{as}} = 3$. The dashed blue line shows an exact numerical computation. The blue shaded area represents the exclusion by the cosmological limit on the neutrino mass sum. Experimental values are taken from [40, 54].

good agreement between the exact numerical computation (dashed blue line) and the result derived from the analytical formulas (solid red line) despite the overall large effects of the Kähler correction.

Although the chosen magnitudes for VEV and coupling strength are not uncommon in flavour model building, they are rather at the verge of their expected range. That is, the value of θ_{13} shown in the plot is close to the maximum that can possibly be achieved using the Kähler corrections alone. The mass range plotted extends to 0.1 eV, but such very large values are at least strongly disfavoured by the cosmological bound derived by Planck, see (III.1.11). The area excluded by this bound is shaded in blue. Moreover, the $\pm 1\sigma$ region around the best fit value for θ_{13} from Table III.3 is shown in the plot as a green shaded band. Choosing m_{ν_1} close to the maximal still allowed value and making the assumptions laid out before, one can thus obtain a θ_{13} that is within 3σ of the best fit value. Even though it does not seem very likely that this effect is the sole explanation of the sizeable value of θ_{13}, the result provides a proof of concept that large contributions even to angles that are zero at first order can be obtained from Kähler corrections.

The other two mixing angles are predicted by the analytical formulas to stay invariant under the Kähler correction considered. Due to higher-order effects, amplified by the large changes in θ_{13}, this is not exactly true, but their changes are still considerably smaller than the changes to θ_{13}. Numerical results for the other two angles are shown in Figure V.2. Taking all results together and comparing the changes with the 3σ regions from Table III.3, one can conclude that, assuming a large coupling value and neutrino masses close to the cosmological bound, one can bring all three angles in rough agreement with experiment. However, it is important to repeat that it seems very unlikely that the A_4 model with Kähler corrections is the correct explanation of the neutrino mixing parameters. The results should rather be seen as a hint to exercise caution when comparing model predictions to experiment without taking into account the corrections discussed here. They are sizeable and can alter

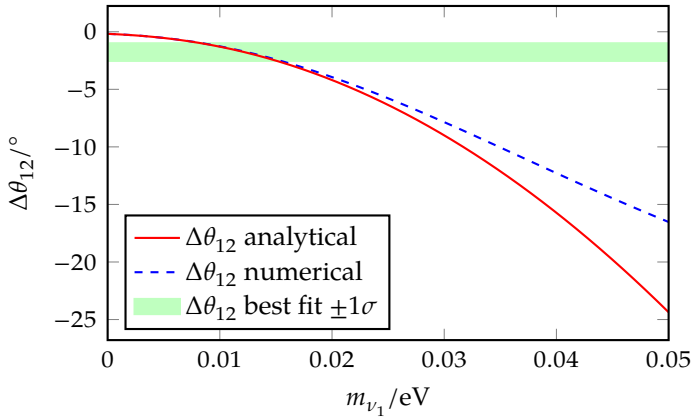


Figure V.3: Correction to θ_{12} in the A_4 model due to the additional Kähler metric contribution $\Delta\hat{\mathcal{K}}_L = \kappa_e^{\mathbf{1}} \frac{|v'|^2}{\Lambda^2} \frac{2}{3} P_{\mathrm{I}}$ in dependence of the lightest neutrino mass m_{ν_1}. The other neutrino masses are fixed by the measured mass differences. The free parameters are set to $|v'|/\Lambda = 0.2$ and $\kappa_e^{\mathbf{1}} = 1/2$. The dashed blue line is an exact numerical computation and the solid red line shows the linear approximation discussed in the text. The green shaded area shows the $\pm1\sigma$ range around the best fit point for θ_{12}. Experimental values are taken from [54].

the model predictions heavily.

To emphasize this point, a second correction is considered in some detail. This correction is due to P_{I}, see e.g. the first term in equation (4.9). The analytical formulas predict a change of θ_{12} of size

$$\Delta\theta_{12} = \kappa_e^{\mathbf{1}} \frac{|v'|^2}{\Lambda^2} \frac{\sqrt{2}}{9} \frac{m_{\nu_1} + m_{\nu_2}}{m_{\nu_1} - m_{\nu_2}} \,. \tag{4.15}$$

There are no contributions due to charged leptons because diagonal corrections to their Kähler metric only change their mass eigenvalues but not the mixing angles. This is due to the chosen basis with diagonal m_e. The resulting change of θ_{12} is plotted in Figure V.3 for $|v'|/\Lambda = 0.2$ and $\kappa_e^{\mathbf{1}} = 1/2$ up to a mass $m_{\nu_1} = 0.05\,\mathrm{eV}$. Despite the relatively small coupling, which does not offset the suppression due to the Clebsch–Gordan coefficients, the corrections are very large. Starting from $m_{\nu_1} = 0$, they drive the angle θ_{12} first through the best fit region shaded in green and then away from it to smaller values. Up to a correction of the order of ten degrees, the analytical formulas and the numerical computation agree well. For even larger values of $\Delta\theta_{12}$, however, the linear approximation made in expressing the change of the angle in terms of its first derivative breaks down and the actual correction is smaller than predicted.

The changes of θ_{13} and θ_{23} due to P_{I} are predicted to be zero by the analytical formulas. Since this is precisely matched by the numerical computation, no plots are shown for these mixing angles.

In contrast to the two cases discussed so far, there are also corrections that do not depend on the neutrino masses. An example is the second term in equation (4.9), i.e. the contribution with the structure of P_{IV}. The analytical formulas for the changes of the mixing angles are

$$\Delta\theta_{12} = \kappa_\nu^{\mathbf{1}} \frac{|v|^2}{\Lambda^2} \frac{\sqrt{2}}{3} \frac{m_\mu^2\, m_\tau^2 - m_e^4}{(m_\mu^2 - m_e^2)\,(m_\tau^2 - m_e^2)} \approx \kappa_\nu^{\mathbf{1}} \frac{|v|^2}{\Lambda^2} \frac{\sqrt{2}}{3} \,, \tag{4.16a}$$

$$\Delta\theta_{13} = \kappa_\nu^{\mathbf{1}} \frac{|v|^2}{\Lambda^2} \frac{\sqrt{2}}{3} \frac{m_e^2 \left(m_\tau^2 - m_\mu^2\right)}{\left(m_\mu^2 - m_e^2\right)\left(m_\tau^2 - m_e^2\right)} \approx \kappa_\nu^{\mathbf{1}} \frac{|v|^2}{\Lambda^2} \frac{\sqrt{2}}{3} \frac{m_e^2}{m_\mu^2} \ll 1\,, \tag{4.16b}$$

$$\Delta\theta_{23} = \kappa_\nu^{\mathbf{1}} \frac{|v|^2}{\Lambda^2} \frac{1}{3} \frac{m_\mu^2 + m_\tau^2}{m_\mu^2 - m_\tau^2} \approx -\kappa_\nu^{\mathbf{1}} \frac{|v|^2}{\Lambda^2} \frac{1}{3}\,. \tag{4.16c}$$

Using again a coupling value of 3 to offset the normalisation of the Clebsch–Gordan coefficients and a VEV-to-scale ratio of 0.2, the changes are thus

$$\Delta\theta_{12} \approx 3.2^\circ\,, \tag{4.17a}$$

$$\Delta\theta_{13} \approx 0^\circ\,, \tag{4.17b}$$

$$\Delta\theta_{23} \approx -2.3^\circ\,, \tag{4.17c}$$

within 10 % agreement of a numerical computation, which also bears out the independence from the neutrino masses.

It should be noted that there is no (theoretical) reason to prefer any one correction over the others. They are all on the same footing theoretically and have to be taken into account when discussing the predictions of the A_4 model. Without any UV completion of this model or any other guide to which higher-dimensional operators can enter the Kähler potential and with which strength, it seems, hence, difficult to make definite predictions. The model can both be made viable again by Kähler corrections or driven away even further from the experimental values. A conclusive answer to the question whether the A_4 model could still qualify as the underlying model of neutrino masses and mixing can thus not be given without further theoretical advances.

Nonetheless, the example computations show that the analytical formulas computed in Section V.3 yield a good approximation to the true changes of the mixing angles due to Kähler corrections for not too large coupling values and not too degenerate neutrino masses, the latter anyway being disfavoured by experiment. The formulas can thus, as intended, be used to quickly estimate the possible corrections to neutrino mixing. To emphasize this point, another example model is discussed in the following section.

V.4.2 Kinetic term corrections to a T′ model

The second example to be discussed is a model by Chen and Mahanthappa [36, 140]. It is a non-supersymmetric SU(5) Grand Unified Theory (GUT) with an additional T′ flavour symmetry. The double tetrahedral group T′ is the double covering group of the tetrahedral group A_4. Its inequivalent irreducible representations are the three singlets, now denoted $\mathbf{1}_{0-2}$, and the triplet $\mathbf{3}$ of A_4 plus three additional doublet representations $\mathbf{2}_0$, $\mathbf{2}_1$ and $\mathbf{2}_2$. More information on the group theory of T′ can be found in Section A.1.2.

Only the details of the model relevant to the kinetic term corrections to neutrino mixing are presented here. All other information, including the mixing pattern for the quark sector, can be found in the original references [36, 140]. The flavon fields, which are all the fields needed to discuss the kinetic term corrections, are shown in Table V.2 together with their T′ representations, their charges under the additional $\mathbb{Z}_{12} \times \mathbb{Z}_{12}$ shaping symmetry and with their vacuum expectation values after flavour symmetry breaking. The fields φ, ξ and φ' are, concerning the kinetic term corrections, the analogues of φ_e and φ_ν, i.e. of the scalar components of Φ_e and Φ_ν, in the A_4 model.

In the quark sector, this flavon content together with the VEV alignment leads to a realistic CKM matrix [36, 140]. Furthermore, the model gives rise to almost tri-bi-maximal neutrino

	φ	φ'	ψ	ψ'	ζ	N	ξ	η
T′	**3**	**3**	$\mathbf{2}_1$	$\mathbf{2}_0$	$\mathbf{1}_2$	$\mathbf{1}_1$	**3**	**1**
$\mathbb{Z}_{12}$	3	2	6	9	9	3	10	10
$\mathbb{Z}_{12}$	3	6	7	8	2	11	0	0
$\langle\cdot\rangle$	$\begin{pmatrix}\varphi_0\\0\\0\end{pmatrix}$	$\begin{pmatrix}\varphi'_0\\\varphi'_0\\\varphi'_0\end{pmatrix}$	$\begin{pmatrix}\psi_0\\0\end{pmatrix}$	$\begin{pmatrix}\psi'_0\\\psi'_0\end{pmatrix}$	ζ_0	N_0	$\begin{pmatrix}\xi_0\\\xi_0\\\xi_0\end{pmatrix}$	η_0

Table V.2: The T′ representations and $\mathbb{Z}_{12} \times \mathbb{Z}_{12}$ charges of all flavon fields of the model by Chen and Mahanthappa [36, 140]. Additionally, the vacuum expectation values are displayed.

	θ_{12}	θ_{13}	θ_{23}	δ_{CP}	δ_e	δ_μ	δ_τ	α_1	α_2
approx. angle/°	33	3	45	227	185	184	180	7	177

Table V.3: Values for the mixing parameters of the T′ model before taking into account kinetic term corrections. The model exhibits approximate tri-bi-maximal mixing with a non-trivial Dirac CP phase δ_{CP}.

mixing. In fact, using the same T′ basis as the original publication, the neutrino mixing matrix is diagonalised by the tri-bi-maximal mixing matrix. However, there are, in contrast to the A_4 model, additional contributions to U_{PMNS} due to a non-diagonal charged lepton mass matrix. The resulting angles and phases are shown in Table V.3. One of the main differences to the A_4 model is that θ_{13} is non-zero even at leading order. Due to the GUT relations, θ_{13} is related to the Cabibbo angle θ_C by

$$\theta_{13} \approx \frac{\theta_C}{3\sqrt{2}}\,. \tag{4.18}$$

Unfortunately, the resulting θ_{13} is not large enough to be phenomenologically viable. It is therefore interesting to investigate whether kinetic term corrections can enhance it sufficiently. Furthermore, the model predicts a non-trivial leptonic Dirac CP phase and an absolute neutrino mass scale with $m_{\nu_1} = 0.0156\,\text{eV}$ and mass-square differences $\Delta m^2_{21} = 8.0 \cdot 10^{-5}\,\text{eV}^2$ and $\Delta m^2_{32} = 2.4 \cdot 10^{-3}\,\text{eV}^2$.

The T′ model is a nice example of a model where no correction to the kinetic terms of the lepton fields which is linear in any flavon can arise. The reason for this is the $\mathbb{Z}_{12} \times \mathbb{Z}_{12}$ shaping symmetry, under at least one factor of which every flavon field is charged. Hence, the lowest-order contributions to the kinetic terms (besides the canonical ones) come from terms quadratic in flavons. Since, as mentioned above, the model contains flavons of the same types as φ_e and φ_ν in the A_4 model, all additional terms discussed in Section V.4.1 also arise here. However, there are new contributions due to the doublet flavons ψ and ψ'. The relevant contraction is

$$\mathbf{2}_i \otimes \mathbf{3} \cong \mathbf{2}_0 \oplus \mathbf{2}_1 \oplus \mathbf{2}_2\,, \qquad i = 0,\,1,\,2\,, \tag{4.19}$$

where **3** is to be replaced by the lepton doublet and $\mathbf{2}_i$ by either ψ or ψ'. The structure of the additional terms is thus

$$\Delta\mathcal{L} \supset \left[(\partial_\mu l) \otimes \psi^{(\prime)}\right]^\dagger_{\mathbf{2}_i} \left[(\partial^\mu l) \otimes \psi^{(\prime)}\right]_{\mathbf{2}_i}\,. \tag{4.20}$$

Using the Clebsch–Gordan coefficients and plugging in the VEVs, one arrives at contributions to the kinetic terms of the form

$$\kappa_{\mathrm{i-vi}} \frac{\left|\psi_0^{(\prime)}\right|^2}{\Lambda^2} \frac{1}{3} \left(\partial_\mu l\right)^T P_{\mathrm{i-vi}} \left(\partial^\mu l\right) + \mathrm{h.\,c.} \tag{4.21}$$

where the VEV of the unprimed field has to be inserted for i to iii and the VEV of the primed field for iv to vi. The factor of one third is again due to the normalisation of the Clebsch–Gordan coefficients. The matrices $P_{\mathrm{i-vi}}$ are defined by

$$P_{\mathrm{i}} \coloneqq \mathrm{diag}\left(0,\, 2,\, 1\right), \tag{4.22a}$$

$$P_{\mathrm{ii}} \coloneqq \mathrm{diag}\left(1,\, 0,\, 2\right), \tag{4.22b}$$

$$P_{\mathrm{iii}} \coloneqq \mathrm{diag}\left(2,\, 1,\, 0\right), \tag{4.22c}$$

$$P_{\mathrm{iv}} \coloneqq \begin{pmatrix} 2 & 1 & -1 \\ 1 & 2 & 0 \\ -1 & 0 & 2 \end{pmatrix}, \tag{4.22d}$$

$$P_{\mathrm{v}} \coloneqq \begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & -1 \\ 1 & -1 & 2 \end{pmatrix}, \tag{4.22e}$$

$$P_{\mathrm{vi}} \coloneqq \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}. \tag{4.22f}$$

Together with the matrices $P_{\mathrm{I-V}}$ from Section V.4.1, these are all structures of additional kinetic terms that arise in the T′ model at quadratic order.

Before discussing the implications of some of these terms, one important difference to the A_4 model has to be discussed. In the A_4 model, the charged lepton mass matrix is diagonal, in accordance with the assumptions made for the derivation of the analytical formulas. This is not the case for the T′ model. Hence, in order to apply the formulas, one has to diagonalise the charged lepton mass matrix first. This does, of course, not affect the initial mixing parameters since they are basis-independent. However, it does affect the non-canonical parts of the kinetic terms. Let the charged lepton matrix be diagonalised by a transformation

$$l \mapsto V\, l \tag{4.23}$$

with V unitary and a similar transformation for the charged lepton singlets. Then the P matrices presented above must be adjusted to

$$\left(\partial_\mu l\right)^\dagger P \left(\partial^\mu l\right) \mapsto \left(V\, \partial_\mu l\right)^\dagger P\, V \left(\partial^\mu l\right) = \left(\partial_\mu l\right)^\dagger \hat{P} \left(\partial^\mu l\right) \tag{4.24}$$

with $\hat{P} \coloneqq V^\dagger P\, V$.

Another difference with respect to the A_4 model is that the neutrino masses are not free parameters but that $m_{\nu_1} = 0.0156\,\mathrm{eV}$ as stated above. Hence, it does not make sense to discuss the dependence of the corrections on the neutrino mass spectrum. The only free parameter is the product of the coupling and the square of the ratio of VEV to scale. Thus, the plots to be discussed below show the dependence of the mixing angles on this quantity up to assumed values of 3 for the coupling and 0.2 for the VEV-to-scale ratio and compare it

to exact numerical computations. Of course, this means that the results from the analytical formulas are straight lines because they are linear approximations.

Since for the T′ model θ_{13} turns out to be too small, even though it is not zero, it is worthwhile to discuss the correction related to the matrix P_{V} again, which in the A_4 case leads to large changes of this angle. The results are shown in Figure V.4. Analytical and numerical results agree reasonably well although for larger values of the coupling the numerical computation deviates from a straight line. The correction is too small to bring θ_{13} into agreement with experiment, even for large values of coupling times VEV suppression. The reason is clear from the comparison with Figure V.1, which also only predicts a change of about 3° for a mass m_{ν_1} of the size present in the T′ model.[11] In principle, there is the possibility that the two contributions by φ' and ξ, respectively, add up, thereby leading to a larger correction to θ_{13}. However, this can be considered a rather remote possibility.

As an example for a correction not present in the A_4 model, the contribution due to P_{vi} to θ_{23} is shown in Figure V.5. Again, analytical and numerical computations are generally in good agreement. The correction turns out not to be very large, which can be understood from the highly non-degenerate neutrino mass spectrum predicted by the model. The corrections to θ_{12} and θ_{13} show the same trend; however, with only one half and one fifth, respectively, of the size of $\Delta\theta_{23}$.

From these examples it can be seen that the T′ model is comparably safe from corrections to the kinetic terms. This is a virtue for the predictivity of the model because the results do not change too much with these additional contributions. However, it is also impossible to make the model viable again by increasing θ_{13} using kinetic term corrections. Both issues are, of course, two sides of the same medal and can be attributed to the small lightest neutrino mass m_{ν_1} and the thus non-degenerate neutrino spectrum. For a way to accommodate a realistic θ_{13} in the T′ model by adding an additional singlet flavon, cf. [141].

V.4.3 A basis of P matrices

Since the analytical formulas derived in Section V.3 are linear approximations, the contributions of different additional kinetic terms can be summed. That is, the additional contributions to the Kähler metric $\hat{\mathcal{K}}$ can be decomposed into a basis of Hermitian matrices, their individual contributions to the mixing angles determined, and the final results summed.[12] One convenient choice of basis is the following:

$$
\begin{aligned}
P_1 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & P_2 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & P_3 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
P_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & P_5 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, & P_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\
P_7 &= \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & P_8 &= \begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \end{pmatrix}, & P_9 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}.
\end{aligned}
\tag{4.25}
$$

In order to gain some intuition on which results are to be expected for which kind of kinetic term correction, one can look at their individual contributions for a certain set of

11 Note that Figure V.1 is, for the reasons outlined above, only an approximation for the T′ model.

12 In fact, this is more or less what the package `KaehlerCorrections` does.

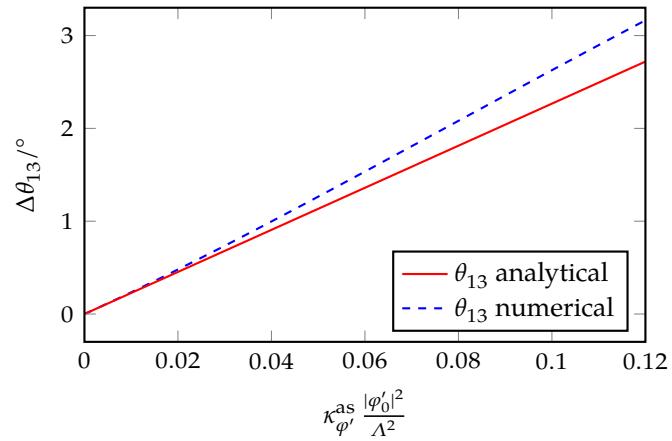


Figure V.4: Correction to θ_{13} in the T′ model due to the additional Kähler metric contribution $\Delta\hat{\mathcal{K}}_L = \kappa^{\text{as}}_{\varphi'} \frac{|\varphi'_0|^2}{\Lambda^2} \sqrt{3}\, P_{\text{V}}$ in dependence of $\kappa^{\text{as}}_{\varphi'} \frac{|\varphi'_0|^2}{\Lambda^2}$. The dashed blue line is an exact numerical computation and the solid red line shows the linear approximation.

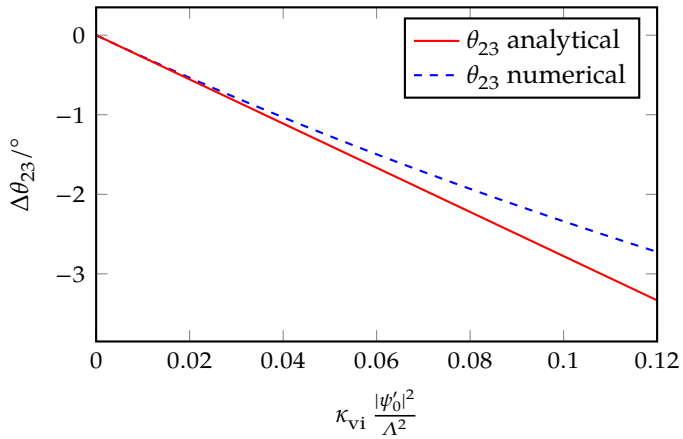


Figure V.5: Correction to θ_{23} in the T′ model due to the additional Kähler metric contribution $\Delta\hat{\mathcal{K}}_L = \kappa_{\text{vi}} \frac{|\psi'_0|^2}{\Lambda^2} \frac{1}{3}\, P_{\text{vi}}$ in dependence of $\kappa_{\text{vi}} \frac{|\psi'_0|^2}{\Lambda^2}$. The dashed blue line is an exact numerical computation and the solid red line shows the linear approximation.

	θ_{12}	θ_{13}	θ_{23}	δ_{CP}	δ_e	δ_μ	δ_τ	α_1	α_2
tri-bi-maximal	$\arctan\frac{1}{\sqrt{2}}$	0	$\frac{\pi}{4}$	–	π	π	0	$2\,\pi$	$2\,\pi$
bi-maximal	$\frac{\pi}{4}$	0	$\frac{\pi}{4}$	–	π	π	0	$2\,\pi$	$2\,\pi$

Table V.4: Tri-bi-maximal and bi-maximal mixing parameters as used for the computation of the corrections for the full basis of P matrices.

	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9
$\Delta\theta_{12}/^\circ$	−0.98	−0.28	0.49	−0.28	0.97	0.49	0	0	0
$\Delta\theta_{13}/^\circ$	0	−0.11	−0.015	0.11	0	0.015	−0.073	0.073	0.011
$\Delta\theta_{23}/^\circ$	0	−0.021	−0.23	0.021	−0.29	0.23	0	0	0

Table V.5: Changes of the mixing angles under Kähler corrections of the form $\Delta K = x_L\, L^\dagger\, P_i\, L$ for $x_L = 0.01$ and $m_{\nu_1} = 0.01\,\text{eV}$ starting from tri-bi-maximal mixing.

initial parameters. Here only contributions due to the left-handed sector are considered, i.e. from Kähler potentials of the form

$$K = L^\dagger\ (1 + x_L\, P_i)\ L + R^\dagger\, R \tag{4.26}$$

or from equivalent kinetic terms in the non-supersymmetric case.

The sets of initial values used are tri-bi-maximal mixing, as obtained from the A_4 model, and bi-maximal mixing. The precise values are compiled in Table V.4. Note that the results depend on all the parameters, i.e. also on Majorana phases and charged lepton phases.

Furthermore, one has to set a specific neutrino mass scale, which is chosen here by setting $m_{\nu_1} = 0.01\,\text{eV}$ and computing the other two masses such that their mass square differences are correct for normal hierarchy.

The last point to be decided is which value of x_L to use. However, whereas the dependence on the masses in non-linear, as seen in Figure V.1, the dependence on x_L is linear. One can hence obtain the result for any desired x_L from the tables by a simple re-scaling. For the tables, $x_L = 0.01$ is used.

Moreover, as already discussed, δ_{CP} is not well defined for $\theta_{13} = 0$, which is true for both tri-bi-maximal and bi-maximal mixing. Hence, the technique using the analyticity of the change of δ_{CP} at zero as described in Section V.4.1 is used to set δ_{CP} in each individual case. This means that the results for two P_i cannot just be summed up to give the correct result for the sum of the P_i since for two different P_i also two different δ_{CP} might be computed, with the real δ_{CP} of the sum being some interpolation of the two results. This is, of course, taken care of in the `KaehlerCorrections` package.

The results following the assumptions made are shown in Table V.5 and Table V.6.

It is interesting to note that the three CP violating matrices $P_{7/8/9}$ only contribute to θ_{13} but not to the other two angles. Generally, the changes to θ_{12} are largest, reaching 1° even for the small neutrino mass scale and small x_L chosen. For a still realistic value of $x_L = 0.1$ or, alternatively, larger m_{ν_1}, the change could easily increase to 10°, in agreement with the situation in the A_4 model depicted in Figure V.3. However, it should be clear that the linear approximation should be used with care for such large corrections because the backreaction becomes non-negligible.

In addition to these tables, which only contain results for fixed m_{ν_i}, one can compute the

	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9
$\Delta\theta_{12}/^\circ$	-1.0	0.20	0.52	0.20	1.0	0.52	0	0	0
$\Delta\theta_{13}/^\circ$	0	-0.12	-0.015	0.12	0	0.015	-0.075	0.075	0.012
$\Delta\theta_{23}/^\circ$	0	-0.022	-0.23	0.022	-0.29	0.23	0	0	0

Table V.6: Changes of the mixing angles under Kähler corrections of the form $\Delta K = x_L\, L^\dagger P_i\, L$ for $x_L = 0.01$ and $m_{\nu_1} = 0.01\,\text{eV}$ starting from bi-maximal mixing.

analytical formulas for a given set of initial mixing parameters for each of the P_i but without specifying neutrino masses. For tri-bi-maximal mixing, the results of this computation are presented in Appendix B. The formulas thus obtained are remarkably simple and, as seen in the examples above, give a good estimate of how large any corrections to mixing angles are.

V.5 Further implications

In this section, two further possible implications of additional Kähler potential terms shall be discussed. The first point to be addressed is the alignment of vacuum expectation values of flavons and its sensitivity to the Kähler corrections. The second topic concerns flavour changing neutral currents (FCNCs) as, making some assumptions about the structure of the soft supersymmetry breaking terms, one can try to obtain information on the size of the Kähler potential couplings from experimental limits on, for example, the decay $\mu^+ \to e^+ + \gamma$.

Note that, whereas the discussion on the kinetic term corrections to the neutrino mixing angles equivalently holds for supersymmetric and non-supersymmetric models, this is not true for the results presented in this section.

V.5.1 Alignment of vacuum expectation values

In models with discrete flavour symmetries, the alignment of vacuum expectation values is often decisive for their predictions. Assuming that the VEVs of flavon fields are dynamically determined by a potential, rather than imposed by hand as is common practice, additional terms could shift the minimum. In particular, highly symmetric solutions like, for example, (v, v, v) for a triplet VEV could be perturbed to something less symmetric like $(v + \Delta v, v, v)$. Symmetric here means that the VEV is invariant under some non-trivial subgroup of the original flavour group, i.e. it does not break the group completely. However, the full set of VEVs has to break the flavour group completely (up to abelian factors) to obtain a realistic spectrum, see also Section III.2. Thus, although each individual VEV might be at a symmetry enhanced point, this symmetry is not a symmetry of the full Lagrangian and cannot protect the VEV from corrections from the superpotential or the Kähler potential. This situation is clearest in so-called direct models, see also Figure III.2, where the flavour symmetry is broken into two different, non-intersecting subgroups in the neutrino and the charged lepton sectors such that the full Lagrangian is not symmetric at all.

Whereas the VEV perturbations by higher-order superpotential terms are often discussed, cf. e.g. the original references [9, 10] on the A_4 model, Kähler corrections are usually ignored without further justification. Hence, the influence of additional Kähler potential terms on the VEV alignment shall briefly be investigated here.

In the following, the simplifying assumption that the flavon sector is independent of any supersymmetry breaking sector is made. This implies, in particular, that F-term VEVs of flavon fields are neglected.

The vacuum expectation values of the flavon fields are determined by minimising the scalar potential (1.8) of the supersymmetric theory. For this to be minimal, two conditions must be fulfilled, where Φ denotes the collection of all chiral superfields and φ their scalar parts:

$$\frac{\partial W}{\partial \Phi_i}(\langle\varphi\rangle) = 0\,, \qquad \forall\, i\,, \qquad (F\text{-term}) \tag{5.1a}$$

$$\mathrm{Re}\left(\frac{\partial K}{\Phi_i}(\langle\varphi\rangle, \langle\varphi^*\rangle) \cdot (T^a \langle\varphi\rangle)_i\right) = 0\,, \qquad \forall\, a\,. \qquad (D\text{-term}) \tag{5.1b}$$

The conditions are independent of the Kähler metric and the real part of the gauge kinetic function although these are both part of the potential because they are positive definite matrices.[13] This also immediately settles the question whether the F-term conditions are affected by a change in the Kähler potential: they are not. To be precise, if the F-term conditions are fulfilled by a VEV $\langle\varphi\rangle$ for a canonical Kähler potential, this stays true for any non-canonical but physical Kähler potential.

However, the Kähler potential enters the D-term conditions in a non-trivial way. Still, the most common case of flavons which are not charged under any gauge symmetry can be solved easily. This is, for example, the case in any model with just the Standard Model gauge symmetry $\mathrm{G_{SM}}$ because the flavons clearly cannot be charged with respect to this symmetry; otherwise, the flavon VEVs would break Standard Model gauge invariance, rendering the model completely unrealistic. Under the assumption that the flavons are not charged under any gauge symmetries, they do not enter the D-term conditions at all as

$$T^a \varphi = 0 \tag{5.2}$$

for non-gauged fields. Hence, one can conclude that the VEV alignment in models with ungauged flavons, e.g. the $\mathrm{A_4}$ model, is not changed at all by the Kähler corrections.

There is a second case which can be solved generally. Assume that an additional gauge symmetry is broken by the VEVs of a set S of chiral superfields, whereas all other fields, denoted by Φ in the following, are either not charged under the additional gauge symmetry or do not obtain a VEV. If, furthermore, the Kähler potential factorises in the form[14]

$$K\left(\Phi, \Phi^\dagger, S, S^\dagger\right) = K_S\left(S^\dagger \mathbb{1}\, S\right) \cdot K_\Phi\left(\Phi, \Phi^\dagger\right)\,, \tag{5.3}$$

the D-term conditions for this new Kähler potential are just a scalar multiple of the conditions for the canonical Kähler potential and, therefore, equivalent. In this case, one can again conclude that the vacuum alignment is not affected at all by the additional Kähler potential contributions. In particular, this is fulfilled if the additional gauge symmetry is only broken by the VEV of a single field, i.e. if there is only one field that is both charged under the additional gauge symmetry and attains a VEV. This applies, for example, to the T′ model discussed in Section V.4.2.

To summarise, the additional contributions to the Kähler potential do usually not affect the vacuum alignment of the flavon fields. They can hence be ignored in most cases when

13 Otherwise the potential would not be bounded below and, hence, unphysical.

14 Note that both K_S and K_Φ should contain a constant term such that there are the usual kinetic terms for all fields.

discussing the VEV alignment of supersymmetric flavour models. In contrast to that, corrections from the superpotential, which are completely unaffected by the present results, should, of course, be taken into account since they can change the phenomenology of a model.

V.5.2 Kähler corrections and FCNCs

One of the drawbacks of supersymmetric models is that soft supersymmetry breaking terms may introduce unwanted flavour changing neutral currents. This happens if the soft masses and the so-called A-terms are not aligned with the mass and Yukawa terms in the matter sector. The problem can be ameliorated, for example, by discrete flavour symmetries [72]. Moreover, the situation can be improved over naive expectations by renormalisation group effects [142].

However, corrections to the Kähler potential by additional flavon interactions like the ones discussed above in the context of neutrino mixing could, in principle, lead to large FCNCs even in models which, without taking into account the corrections, are within experimental limits. To discuss the influence of Kähler corrections, let us assume that the model under consideration does not suffer from dangerous flavour changing neutral currents when all correction terms are set to zero.[15] Furthermore, supersymmetry shall be broken by the F-term vacuum expectation value of a spurion field X, i.e.

$$\langle X \rangle = \theta^2 \langle F_X \rangle \neq 0 \,. \tag{5.4}$$

The terms relevant for the discussion of flavour changing neutral currents at the present level are [138]

$$K \supset L_i^\dagger \, \mathcal{K}^{ij} \, L_j + \frac{1}{\Lambda_{\text{soft}}} \left(X \, L_i^\dagger \, n_L^{ij} \, L_j + \text{h. c.} \right) - \frac{1}{\Lambda_{\text{soft}}^2} \, X^\dagger X \, L_i^\dagger \, k_L^{ij} \, L_j + (L \to R) \,, \tag{5.5a}$$

$$W \supset Y_e^{ij} \, L_i \, R_j \, H_d - \frac{1}{\Lambda_{\text{soft}}} \left(Y_e^X \right)^{ij} \, X \, L_i \, R_j \, H_d \,, \tag{5.5b}$$

where Λ_{soft} is the messenger scale of SUSY breaking and all coupling matrices are functions of the cut-off scale Λ and the flavon superfields. Moreover, the couplings $\mathcal{K}_{L/R}$ and $k_{L/R}$ are Hermitian.

Integrating out the auxiliary fields and replacing the spurion by its VEV, one obtains the soft terms

$$\mathcal{L}_{\text{soft}} \supset -\tilde{l}_i^\dagger \, \left(\widetilde{m}_{\text{LL}}^2 \right)^{ij} \, \tilde{l}_j - \tilde{r}_i^\dagger \, \left(\widetilde{m}_{\text{RR}}^2 \right)^{ij} \, \tilde{r}_j - \left(\tilde{l}_i \, A_{\text{LR}}^{ij} \, \tilde{r}_j + \text{h. c.} \right) \tag{5.6}$$

for the slepton fields $\tilde{l}$ and $\tilde{r}$ with [138]

$$\widetilde{m}_{\text{LL/RR}}^2 := \widetilde{M}^2 \left[k_{L/R} + n_{L/R}^\dagger \, n_{L/R} \right] , \tag{5.7a}$$

$$A_{\text{LR}} := \sqrt{\widetilde{M}^2} \left[Y_e^X + n_L \, Y_e + Y_e \, n_R \right] . \tag{5.7b}$$

Here the scale $\widetilde{M}^2 := |\langle F_X \rangle|^2 / \Lambda_{\text{soft}}^2$ is introduced.

15 This assumption is reasonable because, if a model suffers from FCNCs even before corrections, it also does so afterwards. In fact, these original contributions would be the leading ones and would shadow the influence of any Kähler corrections.

For simplicity, it is assumed that at lowest order

$$\hat{\mathcal{K}}_{L/R} = \mathbb{1}\,, \tag{5.8a}$$
$$n_{L/R} = \eta_{L/R}\,\mathbb{1}\,, \tag{5.8b}$$
$$k_{L/R} = \kappa_{L/R}\,\mathbb{1}\,. \tag{5.8c}$$

This is automatically enforced by the flavour symmetry if all left-handed lepton fields are in a single irreducible representation and, analogously, the right-handed leptons in another irreducible representation. It is then a simple consequence of Schur's lemma (Theorem 9). If the leptons are in reducible representations, the matrices are at least still diagonal if no two generations transform in equivalent representations.

After introducing higher-order terms in the form of contractions of flavon and lepton fields as discussed above for the kinetic terms, all three coupling matrices are perturbed. The new matrices can be written as

$$\hat{\mathcal{K}}_{L/R} = \mathbb{1} - 2\,x\,P_{L/R}\,, \tag{5.9a}$$
$$n_{L/R} = \eta_{L/R}\,\left(\mathbb{1} - 2\,x\,N_{L/R}\right)\,, \tag{5.9b}$$
$$k_{L/R} = \kappa_{L/R}\,\left(\mathbb{1} - 2\,x\,K_{L/R}\right)\,, \tag{5.9c}$$

where the parameter x is supposed to encode the size of the corrections while the matrices $P_{L/R}$, $N_{L/R}$ and $K_{L/R}$ have entries of order unity. Thus, x is usually of the order of the flavon VEVs over the cut-off scale squared, see the discussion in Section V.4.1, and also depends on the unknown couplings in the Kähler potential.

Hence, there are two contributions to the soft masses. One is due to the canonical normalisation of matter fields, i.e. related to $P_{L/R}$, and the other comes directly from the changes of the soft breaking terms, i.e. from $N_{L/R}$ and $K_{L/R}$. To linear order in x the perturbed soft masses are

$$\begin{aligned}\widetilde{m}^2_{\mathrm{LL/RR}} = \widetilde{M}^2 \Big\{ &\left(\kappa_{L/R} + \left|\eta_{L/R}\right|^2\right)\,\mathbb{1} \\ &+ 2\,x\,\left[\kappa_{L/R}\,\left(P_{L/R} - K_{L/R}\right) + \left|\eta_{L/R}\right|^2\,\left(P_{L/R} - N_{L/R} + \mathrm{h.\,c.}\right)\right]\Big\}\,.\end{aligned} \tag{5.10}$$

All additional contributions are, of course, proportional to the small parameter x. In particular, all non-diagonal terms are suppressed by this small quantity, owing to the assumption that there are no zero-th order off-diagonal terms. If there is a relation between the corrections to kinetic terms and to soft terms, they can cancel each other. However, this is generally not to be expected because, even if structurally similar due to the flavour symmetry, there is no reason why their individual coefficients should be the same.

A similar discussion applies to the A-terms. By the assumptions made, all off-diagonal terms are proportional to the small parameter x. However, the phenomenological effects also depend on whether the original A-terms are hierarchical in the sense that, for example, the electron-related terms are smaller than the τ-related terms by a factor of m_e/m_τ. This would be the case, for example, if the mass hierarchy were due to a Froggatt–Nielsen symmetry because in this case the hierarchy of Y_e carries over to Y_e^X.

Inserting the corrected soft terms into formulas like the ones by Gabbiani et al. [143], one can compute the branching fractions for FCNCs as functions of the expansion parameter x and the slepton mass scale. Without any further assumptions on the specific model, it is difficult to make proper quantitative statements. However, it is possible to estimate the order of magnitude needed for the soft masses in order not to violate present bounds on

FCNCs. The decay $\mu^+ \to e^+ + \gamma$ is presently one of the rare decay processes with the best experimental bounds and shall thus be used as an example here. In fact, the result of the MEG collaboration shows that the branching fraction is $\mathrm{Br}(\mu^+ \to e^+ + \gamma) < 5.7 \cdot 10^{-13}$ [71]. Using the formulas from [143], one arrives at the conclusion that for $x \lesssim 0.04$ as assumed in Section V.4, soft masses of the order 2 TeV are safe and, depending on the model details, smaller values might also still be feasible [144].[16] Of course, the limit on the soft masses decreases for smaller x and vice versa. Hence, such limits can either be seen as lower bounds on possible soft masses or upper bounds on the possible size of Kähler corrections.

Fixing the ratios of VEVs to cut-off, one thus obtains information on the otherwise completely unknown size of couplings in the Kähler potential by these considerations.[17] However, it is difficult to interpret these results as limits specifically on the couplings in the Kähler potential that are relevant to neutrino mixing. This is due to the fact that, in addition to the canonical normalisation contributions to FCNCs, which also affect the neutrino mixing, there are direct contributions of the flavons to the soft masses and A-terms, which do not affect the neutrino phenomenology. Without any further assumptions, it is impossible to disentangle the two contributions from each other. Even worse, there is, in principle, the possibility that the two contributions cancel partly, allowing for larger effects in the neutrino sector than would be expected from bounds on FCNCs.

Thus, the only conclusion one can safely draw is that for low TeV-scale SUSY the effects of additional Kähler potential terms can be dangerous and should be taken into account when discussing FCNCs. If soft masses are larger than a few TeVs, the model can be considered safe from Kähler corrections to FCNCs in the sense that, if it is safe ignoring these contributions, bounds are also not violated when taking them properly into account. Without further model assumptions, however, experimental limits on FCNCs are not sufficient to constrain the Kähler potential couplings relevant for neutrino mixing.

V.6 Conclusion of the chapter

The results of this chapter show that kinetic term corrections to neutrino mixing should not be underestimated. Their effects can be large even though the terms responsible are usually suppressed by at least an order of magnitude compared to the canonical kinetic terms. This is particularly important because, for any discrete non-abelian flavour symmetry, one can write down additional contributions to the kinetic terms that cannot be forbidden by any additional symmetry. These are terms that are quadratic in a specific flavon.

The effects of canonical normalisation are similar to renormalisation group effects but can have a more general structure. In particular, there is no reason to assume that effects related to the τ lepton are larger than effects related to the electron, or that the effects are diagonal in a basis with a diagonal charged lepton mass matrix. Moreover, effects due to additional kinetic terms are not loop suppressed but depend on the ratio of flavon vacuum expectation values to the new physics scale, which can be very sizeable in flavour models. Note that, as already explained in Section V.1, the discussion applies to supersymmetric and non-supersymmetric models alike.

The analytical formulas developed here are made available as the MATHEMATICA package

16 At the time of the original publication [2], only older and, hence, weaker limits on this branching fraction were available. Thus, the new limits are stronger than the ones originally presented.

17 For a very recent discussion of the influence of general Kähler potentials on flavour changing neutral currents in M-theory models, cf. [145].

`KaehlerCorrections`, which can be found online.[18] This package can be used to easily estimate the effects of kinetic term corrections directly on the mixing parameters. The formulas only depend on the mass and mixing parameters obtained by ignoring the additional terms, i.e. on their naive results. Their analytical expressions show that the effects of corrections to the right-handed kinetic terms are more or less negligible due to the large mass hierarchy among the charged leptons. By the same reasoning the effects from the left-handed kinetic terms are largest for almost degenerate neutrino masses. The validity of these statements and of the formulas in general was established using two example models based on the groups A_4 and T′, respectively, by comparing the approximate analytical results to an exact numerical computation.

The corrections to the Kähler potential were also shown not to be a danger for the VEV alignment in supersymmetric models in most practical cases. In contrast to that, their effect on flavour changing neutral currents in such models cannot safely be neglected without further model assumptions. An estimate of the influence of flavon induced Kähler corrections to the rate of the decay $\mu^+ \to e^+ + \gamma$ does, however, not indicate any severe problems for soft masses slightly above the TeV-scale [144].

Summarising, one can conclude that, on the one hand, kinetic term corrections provide more freedom for model building. It is, for example, possible to revive models that seem to have been ruled out by experiment using these additional contributions to neutrino mixing. Indeed, it was shown that in the A_4 model by Altarelli and Feruglio [9, 10], one can, in principle, raise the angle θ_{13} to about 8°, which is still feasible.

On the other hand, the corrections constitute a large arbitrariness in flavour model building. The size of the effects depends on the couplings in the Kähler potential or the additional kinetic terms about which little is known. It seems thus very important to gain more insight into the structure of Kähler potentials and kinetic terms by constructing consistent UV completions for such flavour models. Further possible avenues to obtain more information on Kähler potentials are computations using wave function overlaps [146, 147] and comparisons with cases where the Kähler potential is partly known [148]. An important implication of the arbitrariness is that scans, cf. e.g. [149, 150], over neutrino flavour models that do not take into account the kinetic term corrections probably largely underestimate the number of viable models because of the large additional theoretical uncertainties.

18 http://einrichtungen.ph.tum.de/T30e/codes/KaehlerCorrections

VI Breaking compact classical Lie groups to finite subgroups

Explaining the flavour structure of the Standard Model using discrete non-abelian symmetries is, in a sense, only a first step. Subsequently, one would, of course, also like to explain the origin of these symmetries. As already mentioned, this problem is amplified because global symmetries are believed to be broken by gravitational effects [12, 13]. One possible consistent origin of these symmetries is provided by string theory [62, 98–100]. However, there is another, more bottom-up possibility to obtain discrete symmetries that are protected from violation by gravitational effects: spontaneous breaking of a (non-anomalous) continuous gauge group like $\mathrm{SU}(N)$ [61]. Symmetries of this kind are known as discrete gauge symmetries.

The aim of this chapter is to aid the construction of models where a discrete non-abelian symmetry emerges from the spontaneous breaking of a continuous symmetry, i.e. from breaking Lie groups to finite subgroups. This is only possible if there is a non-trivial irreducible representation of the Lie group that contains a trivial singlet of the subgroup. A vacuum expectation value of this component may then break the Lie group to the desired subgroup. A procedure is thus outlined here for the decompositions of Lie group representations into irreducible representations of a given subgroup. The resulting routines are also implemented in the Mathematica [11] package `DecomposeLGReps`.

The decomposition of a representation of a finite group G into representations of a subgroup $H \subset G$ proceeds via the scalar product of characters, see Section II.4. The branching rules can be computed using the following algorithm. Given a representation $\boldsymbol{R}$ of G, restrict it to the desired subgroup H. Then the character scalar product of $\boldsymbol{R}$ with an irreducible representation $\boldsymbol{r}_i$ of H yields the multiplicity μ_i of $\boldsymbol{r}_i$ in $\boldsymbol{R}$,

$$\mu_i = (\chi_{\boldsymbol{r}_i}, \chi_{\boldsymbol{R}}|_H) = \frac{1}{|H|} \sum_{h \in H} \chi_{\boldsymbol{r}_i}(h)^* \, \chi_{\boldsymbol{R}}(h) \,. \tag{0.1}$$

The same technique can, in principle, be used for Lie groups as long as their dimension is finite. However, whereas character tables of finite groups contain all information needed to go through this procedure, it is clearly impossible to compile all the necessary information for Lie groups; the character table had to be infinitely large.

Hence, previous studies used different methods to compute the branching rules. A first possibility is using the fact that each Lie group representation can be obtained from the tensor product of fundamental representations[1] as in [111, 151]. A second option is working

* Some of the results presented in this chapter have already been communicated in [6].

1 So-called spinor representation of $\mathrm{SO}(N)$ are an exception, see also Section VI.1 below.

with explicit realisations of the Lie group representations [152]. Both approaches cannot easily be generalised to larger Lie group representations or larger rank Lie groups. In another approach that also highlights the connection between spontaneous and explicit symmetry breaking, Merle and Zwicky [153] used an algorithm based on group invariants and provided a MATHEMATICA package implementing the algorithm for SU(3). Again this is not easily generalised, and the method relies on rather advanced notions of invariant theory. Similar considerations also lead to the so-called generating functions for subgroup scalars compiled in [154]; the focus of [154], however, is mainly on Lie subgroups of Lie groups.

To overcome these limitations, the present work uses the standard technique of the character scalar product (0.1) and computes the characters on the fly with MATHEMATICA using what is called the Weyl character formula [155] (for more modern treatments see, for example, [18, 115]). Note that, since the sum in (0.1) runs over the finite number of elements of the subgroup, only a finite number of Lie group characters has to be computed. Thus, the procedure, in principle, allows the computation of branching rules for all compact Lie groups and arbitrary finite subgroups thereof. The associated MATHEMATICA package `DecomposeLGReps` implementing the formulas for the classical Lie groups U(N), SU(N), SO(N) and USp($2N$) can be found online.[2]

Of course, there remain some general issues with this type of model building. For example, the VEV of the singlet component of the Lie group representation under consideration may be left invariant by a larger number of transformations than the desired subgroup, i.e. the subgroup might not be a maximal invariant subgroup. Unfortunately, there is no general theory that exposes whether this is the case or not; hence, this question has to be settled in each case individually, e.g. by examining the subgroup tree [153] or by constructing the actual representation matrices [151, 152]. Furthermore, it is, in general, difficult to write down a potential giving rise to the desired VEV dynamically, at least if one does not want to resort to supersymmetry and driving fields. These caveats notwithstanding, knowledge of candidate representations for the desired breaking is of great help in model building. Moreover, as shown below, in some cases one can discern patterns in the branching rules that allow to make general statements about models embodying this breaking.

In the following, first, criteria for a finite group to be a subgroup of a compact classical Lie group are compiled in Section VI.1. Then Section VI.2 explains the technical details of the computation, i.e. the connection between Lie algebra and Lie group characters and the Weyl character formula. The MATHEMATICA package `DecomposeLGReps` implementing this procedure is briefly presented in Section VI.3. Finally, in Section VI.4, some examples are given for the applicability of the package, and some general results for various small finite groups are derived.

VI.1 Subgroups of compact classical Lie groups

The purpose of this section is to state criteria for a finite group H to be a subgroup of any of the compact classical Lie groups U(N), SU(N), SO(N) and USp($2N$). In fact, the simplest case is the one of the unitary group U(N) because any finite-dimensional representation of a compact group is equivalent to a unitary representation, see Theorem 7.

The criterion used here is that H is a subgroup of U(N) if and only if it has a faithful representation of dimension N.

2 http://einrichtungen.ph.tum.de/T30e/codes/DecomposeLGReps

To see this, let H have a faithful unitary representation $\boldsymbol{R}$ of dimension N,

$$\boldsymbol{R}: \quad H \quad \rightarrow \quad \{N \times N \text{ unitary matrices}\} \quad , \tag{1.1}$$

and let $\boldsymbol{N}$ be the fundamental representation of $\mathrm{U}(N)$,

$$\boldsymbol{N}: \quad \mathrm{U}(N) \quad \rightarrow \quad \{N \times N \text{ unitary matrices}\} \quad , \tag{1.2}$$

which is a bijection. Then the map

$$\boldsymbol{N}^{-1} \circ \boldsymbol{R}: \quad H \quad \rightarrow \quad \mathrm{U}(N) \tag{1.3}$$

is an injective group homomorphism that embeds H into $\mathrm{U}(N)$ as a subgroup.

Now let H be a subgroup of $\mathrm{U}(N)$. Then there exists an embedding i of H into $\mathrm{U}(N)$,

$$i: \quad H \quad \rightarrow \quad \mathrm{U}(N) \quad , \tag{1.4}$$

where i is an injective group homomorphism. Using this map one can define a faithful representation $\boldsymbol{R}'$ of H by

$$\boldsymbol{R}' := \boldsymbol{N} \circ i \, , \tag{1.5}$$

which has dimension N. This concludes the proof of the subgroup criterion for $\mathrm{U}(N)$.

The same arguments go through for the other compact classical Lie groups if, additionally, $\det \rho_{\boldsymbol{R}}(g) = 1$ for $\mathrm{SU}(N)$, $\det \rho_{\boldsymbol{R}}(g) = 1$ and for some choice of basis $\rho_{\boldsymbol{R}}(g) \in \mathbb{R}^{N \times N}$ for $\mathrm{SO}(N)$ and $\rho_{\boldsymbol{R}}(g) \in \mathrm{Sp}(2N, \mathbb{C})$ for $\mathrm{USp}(2N)$.

For works on subgroups of the probably most relevant Lie groups for model building, $\mathrm{SU}(3)$ and $\mathrm{SO}(3)$, see [58, 73, 74, 156], and for a general overview of popular groups for model building, see [57].

One further important remark concerns the notation for Lie group representations used here. An irreducible representation of a Lie group is labelled by the Dynkin labels $\Lambda = (\Lambda^1, \Lambda^2, \ldots, \Lambda^r)$ of the highest weight of its associated Lie algebra representation. This correspondence between Lie group and Lie algebra representations is only one-to-one for simply connected Lie groups, e.g. for $\mathrm{SU}(N)$ and $\mathrm{USp}(2N)$ (cf. [115]). However, $\mathrm{SO}(N)$ is not simply connected and has as universal covering group $\mathrm{Spin}(N)$, e.g. the universal covering group of $\mathrm{SO}(3)$ is $\mathrm{Spin}(3)$ which is isomorphic to $\mathrm{SU}(2)$. Thus, for the present approach one has to distinguish the groups $\mathrm{SO}(N)$ and $\mathrm{Spin}(N)$ carefully in contrast to common practice in physics. In fact, the N-dimensional fundamental representation of $\mathrm{SO}(N)$ is not a faithful representation for $\mathrm{Spin}(N)$. Therefore, the procedure described above really embeds the finite group into $\mathrm{SO}(N)$ and not into $\mathrm{Spin}(N)$. Branching rules are, hence, only computed for non-spinorial representations, i.e. for representations of $\mathrm{SO}(2N+1)$ whose last Dynkin label components Λ^N are even integers and for representations of $\mathrm{SO}(2N)$ with $\Lambda^{N-1} + \Lambda^N$ even.

VI.2 Lie group characters

This section explains the details of the computation of Lie group characters using the Weyl character formula. It is structured as follows. First, the connection of Lie group and Lie algebra characters is reviewed, and the Weyl character formula for the computation of Lie algebra characters in its modern formulation is introduced. Then, after clarifying some notational issues, the Weyl character formulas for the classical Lie groups are presented in two formulations due to Weyl, which are for the present purposes more useful than the general formula mentioned before.

VI.2.1 Lie group and Lie algebra characters

As already explained in Section II.4, the definition of a group character is not limited to finite groups. In fact, the character χ_Λ of a finite-dimensional highest-weight representation of some finite-dimensional Lie group L is defined in the same way, namely

$$\chi_\Lambda(g) := \mathrm{tr}(\rho_\Lambda(g))\,, \qquad \forall g \in L\,, \tag{2.1}$$

where ρ_Λ is a matrix realisation of the representation with highest weight Λ [115]. The characters are again class-functions, i.e. constant on conjugacy classes.

It is important to note that for semi-simple Lie groups any group element g is conjugate to an element $g_\circ$ of a maximal torus, i.e. of a subgroup with the Cartan sub-algebra of the Lie algebra $\mathfrak{l}$ of L as Lie algebra. In other words: each group element can be diagonalised by an inner automorphism [115]. This leads to a relation between so-called Lie algebra characters ch_Λ and the desired Lie group characters χ_Λ. Lie algebra characters ch_Λ are, in principle, defined as the formal generating function [115]

$$\mathrm{ch}_\Lambda := \sum_{\lambda'} \mathrm{mult}_\Lambda(\lambda')\ \mathrm{e}^{\lambda'}\,, \tag{2.2}$$

where the sum runs over all weights of the representation defined by Λ and $\mathrm{mult}_\Lambda(\lambda')$ is the multiplicity of λ' in the weight diagram. They can also be viewed as functions from weight space to the complex numbers by interpreting the action of the exponentials on a weight λ as

$$\mathrm{e}^{\lambda'}(\lambda) := \mathrm{e}^{(\lambda',\,\lambda)}\,, \tag{2.3}$$

where the parenthesis denote the scalar product on weight space. This is given by

$$(\lambda',\,\lambda) := \lambda'^i\, G_{ij}\, \lambda^j \tag{2.4}$$

where G_{ij} denotes the metric on weight space, whose inverse fulfils

$$G^{ij} := \kappa(H^i,\,H^j) \tag{2.5}$$

for the Cartan sub-algebra generators H^i associated to the simple roots in the Chevalley–Serre basis, and where upper indices on weights refer to their components in Dynkin basis, i.e. their Dynkin labels [115]. The Killing form κ can be defined via

$$\kappa(x,\,y) := \mathrm{tr}(\mathbf{adj}(x)\,\mathbf{adj}(y)) = \frac{\ell(\mathbf{adj})}{\ell(\Lambda)}\ \mathrm{tr}\,(\boldsymbol{R}_\Lambda(x)\,\boldsymbol{R}_\Lambda(y)) \tag{2.6}$$

for elements x and y of the Lie algebra $\mathfrak{l}$, where **adj** denotes the adjoint representation and ℓ the Dynkin index.

The relation to Lie group characters is due to the fact that, for each element $g_\circ$ of a maximal torus of a compact Lie group L, one can find an element h of the Cartan sub-algebra of the Lie algebra of L such that $\exp h = g_\circ$. The Lie algebra character $\mathrm{ch}_\Lambda(h)$ of this element equals the Lie group character of g [115],

$$\mathrm{ch}_\Lambda(h) = \chi_\Lambda(\exp h) = \chi_\Lambda(g_\circ) = \chi_\Lambda(g)\,, \tag{2.7}$$

where the last equality follows because χ_Λ is a class-function and because $g_\circ$ is in the same conjugacy class as g.

$\mathfrak{l}$	W	$\lvert W\rvert$
A_r	S_{r+1}	$(r+1)!$
B_r	$\mathbb{Z}_2^r \rtimes \mathrm{S}_r$	$2^r\, r!$
C_r	$\mathbb{Z}_2^r \rtimes \mathrm{S}_r$	$2^r\, r!$
D_r	$\mathbb{Z}_2^{r-1} \rtimes \mathrm{S}_r$	$2^{r-1}\, r!$

Table VI.1: This table is a partial reproduction of [115, (10.29)] and shows the group structures and orders of the Weyl groups of the classical Lie algebras.

It is, hence, possible to compute all Lie group characters using this equivalence with Lie algebra characters given a formula for the latter. In fact, there is a closed formula for Lie algebra characters called Weyl character formula, which in its modern form is given by [115]

$$\mathrm{ch}_\Lambda(\lambda) = \frac{\sum_{w\in W} \mathrm{sign}(w)\ \mathrm{e}^{(w(\Lambda+\rho),\,\lambda)}}{\sum_{w\in W} \mathrm{sign}(w)\ \mathrm{e}^{(w(\rho),\,\lambda)}}\,. \tag{2.8}$$

This formula requires some explanation. First of all, the sums run over all elements of the Weyl group W. This is the group generated by all reflections in weight space at planes orthogonal to the simple roots, i.e. it is generated by all so-called Householder transformations corresponding to the simple roots. The sign of an element w of the Weyl group is defined as $\mathrm{sign}(w) := (-1)^{\mathrm{length}(w)}$, where the length of an element is the (unique) minimal number of reflections defined by simple roots that is needed to generate the reflection w. The structures of the Weyl groups of the classical Lie algebras are shown in Table VI.1. Moreover, ρ denotes the Weyl vector of the Lie algebra and is given by half the sum of the positive roots,

$$\rho := \frac{1}{2}\sum_{\alpha>0} \alpha\,. \tag{2.9}$$

It has components $\rho^i = 1$ for all $i = 1, \dots, \mathrm{rank}\,\mathfrak{l}$ in Dynkin basis.

VI.2.2 Notation for the Weyl character formulas in terms of eigenvalues

The Weyl character formula is finally applied to group elements that are also elements of the finite subgroup in order to compute the branching rules using the character scalar product (0.1). In the case of embeddings as described in Section VI.1, these Lie group elements g are not specified by weights but by an explicit representation matrix $\rho_N(g)$ in the fundamental representation. One possibility to proceed is to compute the corresponding weight for each group element. To this end, the representation matrix $\rho_\Lambda(g)$ is diagonalised and the logarithm of the resulting diagonal matrix $\rho_\Lambda^{\mathrm{diag}}(g)$ is projected onto the generators of the Cartan sub-algebra using the Killing form of the Lie algebra,

$$\lambda^i = \kappa\left(\log \rho_\Lambda^{\mathrm{diag}}(g),\, H^i\right) = \kappa\left(\mathrm{diag}\left(\log \varepsilon_j(g)\right),\, H^i\right)\,, \tag{2.10}$$

where $\varepsilon_j(g)$ is the j-th eigenvalue of the group element g. This yields the correct result because

$$\lambda_i = \kappa\left(\lambda_k H^k,\, H^l\right)\, G_{li}\,. \tag{2.11}$$

The resulting weight λ can now be plugged into equation (2.8) to compute the character.

Instead of first translating the explicit representation matrices of the subgroup into the language of weights, one can also compute the characters directly in terms of their eigenvalues $\varepsilon_i(g)$ [18, 155, 157]. In this case, the irreducible Lie group representation whose character is to be computed is conventionally not labelled by Dynkin labels but by its so-called partition, a notation related to Young tableaux. For SU(N), i.e. Lie algebra $A_{r=N-1}$, the relation of Dynkin labels $\Lambda = (\Lambda^1, \Lambda^2, \dots, \Lambda^{N-1})$ to partitions can be understood in the following way. The Dynkin label component Λ^i is the number of columns with i boxes in the Young tableau corresponding to Λ. The partition is then the list of row lengths f_i of the Young tableau, which can be computed from the Dynkin labels by

$$f_i := \sum_{k=i}^{N-1} \Lambda^k \,, \qquad i = 1, \dots, N-1 \,, \tag{2.12}$$

and which results naturally in the ordering $f_i \geq f_{i+1}$ [18, 157].

Partitions are also the conventional way to label irreducible representations of U(N) [155]. However, in this case an additional integer f_N has to be specified. Furthermore, all $f_{i \leq N-1}$ as computed with the formula above must be increased by this f_N. Restricting a representation from U(N) to its SU(N) subgroup, all representations differing only in this global shift are identical and f_N can be set to zero without loss of generality.

For representations Λ of the symplectic group USp($2N$), i.e. Lie algebra $C_{r=N}$, the N labels f_i of the corresponding Young tableau are again obtained by equation (2.12) with the sum extending up to N [18].

The definition of Young tableaux and partitions for orthogonal groups is more complicated and not unique; thus, one has to be careful when comparing different approaches. In addition to that, one has to distinguish SO($2N$), i.e. Lie algebra $D_{r=N}$, and SO($2N+1$), i.e. Lie algebra $B_{r=N}$. We adopt the conventions of [18, 157].[3] Hence, the partition corresponding to Λ is obtained from

$$f_i := \sum_{k=i}^{N-1} \Lambda^k + \frac{\Lambda^N}{2} \,, \qquad i = 1, \dots, N \,, \qquad \text{for SO}(2N+1) \text{ and} \tag{2.13a}$$

$$f_i := \sum_{k=i}^{N-2} \Lambda^k + \frac{\Lambda^{N-1} + \Lambda^N}{2} \,, \quad i = 1, \dots, N-1 \,, \quad f_N := \frac{\Lambda^N - \Lambda^{N-1}}{2} \,, \quad \text{for SO}(2N), \tag{2.13b}$$

where the sums are set to zero if i is larger than their upper limit. All f_i are integers for non-spinorial representations but half-integer for spinor representations. This does not pose any problem for the present approach since only subgroups of SO(N) are considered, and, therefore, only non-spinorial representations are allowed as input.

It turns out to be convenient to furthermore introduce the abbreviation

$$\ell_i := f_i - i + N \,, \qquad i = 1, \dots, N \,, \tag{2.14}$$

setting $f_N := 0$ for SU(N).

VI.2.3 The Weyl character formulas in terms of eigenvalues

After introducing this notation, the character formulas simply take the form of determinants. Using the simplest case of SU(N) as an example, this can be seen as follows. The main

3 The conventions by Weyl [155] differ only slightly from the other two. He uses the absolute value of f_N for SO($2N$) and adds a prime to distinguish between representations with positive and negative f_N.

observation is that the sum over the Weyl group of the signum of the Weyl group elements times an exponential resembles, the Weyl group of SU(N) being S_N, the Leibniz formula for the determinant of a matrix, which is

$$\det A = \sum_{\sigma\in S_n} \operatorname{sign}(\sigma) \prod_{i=1}^{n} A_{i,\sigma(i)} \,. \tag{2.15}$$

First of all, one has to determine the weight of a given group element g. The generators of the Cartan sub-algebra in the Cartan–Weyl basis are

$$(H^i)_{kl} = \delta_{k,i}\,\delta_{l,i} - \delta_{k,i+1}\,\delta_{l,i+1} \tag{2.16}$$

leading to weight components

$$\lambda^i = \operatorname{tr}\left(\operatorname{diag}\left(\log\varepsilon_j(g)\right) H^i\right) = \log\left(\frac{\varepsilon_i(g)}{\varepsilon_{i+1}(g)}\right). \tag{2.17}$$

The Weyl group is represented most simply not in the Dynkin basis but in the orthogonal basis of weight space, where it is just a permutation of the components. The components of weights are translated from the Dynkin basis to the orthogonal basis by the following formula,

$$\tilde\lambda^i = \sum_{j=i}^{r} \lambda^j - \frac{1}{r+1}\sum_{j=1}^{r} j\,\lambda^j \,, \qquad i = 1,\dots,r+1\,, \tag{2.18}$$

where the first sum is set to zero for $i = r+1$. Note that the weight space is now embedded into $\mathbb{R}^{r+1}$. Hence, the weights of the group element g in the orthogonal basis are

$$\tilde\lambda^i = \log\left(\frac{\varepsilon_i(g)}{\varepsilon_{r+1}(g)}\right) - \frac{1}{r+1}\log\left(\frac{1}{\varepsilon_{r+1}(g)^{r+1}}\right) = \log\left(\varepsilon_i(g)\right), \qquad i = 1,\dots,r+1\,, \tag{2.19}$$

i.e. just the logarithms of the eigenvalues. Here, it is used that the determinant of the matrix and, thus, the product of its eigenvalues is one. The Weyl vector in the orthogonal basis is

$$\tilde\rho^i = \frac{r}{2} + 1 - i\,, \qquad i = 1,\dots,r+1\,. \tag{2.20}$$

This shows that the denominator of the Weyl character formula (2.8) is, in fact,

$$\sum_{w\in W} \operatorname{sign}(w) \prod_{i=1}^{r+1} \varepsilon_i^{r/2+1-w(i)} = \sum_{\sigma\in S_{r+1}} \operatorname{sign}(\sigma) \prod_{i=1}^{r+1} \varepsilon_i^{r/2+1-\sigma(i)} = \det\left[\varepsilon_i^{r/2+1-j}\right]_{ij}. \tag{2.21}$$

Here, $[A]_{ij}$ is the $n\times n$ matrix A with entries labelled by $i,j = 1,\dots,n$, and $\det[A]_{ij}$ is its determinant. In the numerator, the exponent is changed due to the additional highest weight Λ of the representation under consideration,

$$\begin{aligned}\sum_{w\in W} \operatorname{sign}(w) \prod_{i=1}^{r+1} \varepsilon_i^{\sum_{k=w(i)}^{r}\Lambda^k - \frac{1}{r+1}\sum_{k=1}^{r} k\,\Lambda^k + r/2+1-w(i)} \\ = \det\left[\varepsilon_i^{\sum_{k=j}^{r}\Lambda^k - \frac{1}{r+1}\sum_{k=1}^{r} k\,\Lambda^k + r/2+1-j}\right]_{ij}.\end{aligned} \tag{2.22}$$

In both numerator and denominator constant, i.e. j-independent, parts of the exponent drop out because the product of all eigenvalues is one. Hence, one can write the final result for the Weyl character formula for $\mathrm{SU}(N)$ in terms of the eigenvalues $\varepsilon_i(g)$ of a group element g using the notation introduced above as [155]

$$\chi_\Lambda(g) = \frac{\det\left[\varepsilon_i^{\ell_j}(g)\right]_{ij}}{\det\left[\varepsilon_i^{N-j}(g)\right]_{ij}}\,. \tag{2.23}$$

This expression is also called a Schur polynomial [18]. In fact, the denominator can be simplified because it is just a Vandermonde determinant, yielding

$$\chi_\Lambda(g) = \frac{\det\left[\varepsilon_i^{\ell_j}(g)\right]_{ij}}{\prod_{i<j}\left(\varepsilon_i(g)-\varepsilon_j(g)\right)}\,. \tag{2.24}$$

In fact, this formula also holds for $\mathrm{U}(N)$ [155].

The other compact classical Lie groups can be treated similarly. However, in all these cases only half of the eigenvalues are independent because they always come in complex conjugate pairs.[4] Hence, for all groups besides the unitary groups, only one eigenvalue of each pair is to be used in the formulas below such that their number matches the rank of the Lie algebra. The formulas for all compact classical Lie groups are then [18, 155]

$$\chi_\Lambda(g) = \frac{\det\left[\varepsilon_i^{\ell_j}(g)\right]_{ij}}{\prod_{i<j}\left(\varepsilon_i(g)-\varepsilon_j(g)\right)} \qquad \text{for } (\mathrm{S})\mathrm{U}(N), \tag{2.25a}$$

$$\chi_\Lambda(g) = \frac{\det\left[\varepsilon_i^{\ell_j+1}(g)-\varepsilon_i^{-\ell_j-1}(g)\right]_{ij}}{\det\left[\varepsilon_i^{N+1-j}(g)-\varepsilon_i^{-N-1+j}(g)\right]_{ij}} \qquad \text{for } \mathrm{USp}(2N), \tag{2.25b}$$

$$\chi_\Lambda(g) = \frac{\det\left[\varepsilon_i^{\ell_j+1/2}(g)-\varepsilon_i^{-\ell_j-1/2}(g)\right]_{ij}}{\det\left[\varepsilon_i^{N+1/2-j}(g)-\varepsilon_i^{-N-1/2+j}(g)\right]_{ij}} \qquad \text{for } \mathrm{SO}(2N+1), \tag{2.25c}$$

$$\chi_\Lambda(g) = \frac{\det\left[\varepsilon_i^{\ell_j}(g)+\varepsilon_i^{-\ell_j}(g)\right]_{ij}+\det\left[\varepsilon_i^{\ell_j}(g)-\varepsilon_i^{-\ell_j}(g)\right]_{ij}}{\det\left[\varepsilon_i^{N-j}(g)+\varepsilon_i^{-N+j}(g)\right]_{ij}} \qquad \text{for } \mathrm{SO}(2N). \tag{2.25d}$$

These formulas are implemented in the MATHEMATICA package `DecomposeLGReps`.

Unfortunately, there is a computational difficulty because all determinants are zero if any two eigenvalues coincide. This can be most easily seen in the case of $\mathrm{SU}(N)$, where the Vandermonde determinant clearly vanishes for two identical eigenvalues. Fortunately, this is just a removable discontinuity. In the original formula (2.8) this can be ameliorated by adding a multiple of the Weyl vector $t\cdot\rho$ to the weight λ and taking the limit $t\to 0$ after computing the determinant. In (2.25) the same can be achieved by the replacement $\varepsilon_j \to \varepsilon_j\,\mathrm{e}^{\mathrm{i}\,jt}$ and the limit $t\to 0$.

4 Matrices of $\mathrm{SO}(2N+1)$ have an additional eigenvalue $+1$ which also has to be omitted.

The formulas (2.25) are computationally rather demanding because of the possibly large determinants. Computation time should roughly grow as $(r+1)!$, where r is the rank of the Lie group. However, for the ranks of Lie groups usually used in model building this is not a major concern.

A big advantage of the formulas (2.25), however, is that they are closed, i.e. they do not involve any recursion in contrast to, for example, the Freudenthal formula [115]. Hence, they can be used to derive general properties for subgroups of classical Lie groups, see Section VI.4 below.

VI.2.4 An alternative formulation of the Weyl character formulas

If one only needs a result for fixed integer Dynkin labels, a second form of the character formulas can be advantageous. This form circumvents the limit procedure, which, otherwise, considerably slows down the computation. It can be derived using a correspondence between Schur polynomials and determinants of complete homogeneous symmetric polynomials h_i, which are defined by

$$\frac{1}{\prod_i (1 - z\, x_i)} =: \sum_j h_j(x_i)\, z^j\,, \tag{2.26}$$

see [18, 155]. In the present case the polynomials h_i are to be evaluated at the eigenvalues of the representation matrix. In fact, the quantities from which the characters can be computed are the coefficients p_i of the generating function for one divided by the characteristic polynomial of this matrix [18, 155],

$$\frac{1}{\det(\mathbb{1} - z\,\rho_\Lambda(g))} = \frac{1}{\prod_i (1 - z\,\varepsilon_i(g))} = \sum_j h_j(\varepsilon_i(g))\, z^j =: \sum_j p_j(g)\, z^j\,. \tag{2.27}$$

The final formulas for the characters of $\mathrm{U}(N)$, $\mathrm{SU}(N)$ and $\mathrm{USp}(2N)$ are given by [155]

$$\chi_\Lambda(g) = \det\left[p_{\ell_i - N + j}(g)\right]_{ij} \qquad \text{for } \mathrm{U}(N) \text{ and } \mathrm{SU}(N), \tag{2.28a}$$

$$\chi_\Lambda(g) = \frac{1}{2}\det\left[p_{\ell_i - N + j}(g) + p_{\ell_i - N - j + 2}(g)\right]_{ij} \qquad \text{for } \mathrm{USp}(2N). \tag{2.28b}$$

Formulas for $\mathrm{SO}(N)$ cannot be found in [155], but for $\mathrm{O}(2N)$ and $\mathrm{O}(2N+1)$

$$\chi_\Lambda(g) = \det\left[p_{\ell_i - N + j}(g) - p_{\ell_i - N - j}(g)\right]_{ij}. \tag{2.29}$$

The irreducible representations of $\mathrm{SO}(2N+1)$ and $\mathrm{O}(2N+1)$ coincide such that the character formula for $\mathrm{O}(2N+1)$ can also be used for $\mathrm{SO}(2N+1)$. However, only irreducible representations of $\mathrm{SO}(2N)$ whose last two Dynkin labels are equal are also irreducible representations of $\mathrm{O}(2N)$, in which case the characters are again identical. Irreducible representations of $\mathrm{SO}(2N)$ with Dynkin labels $\Lambda^{N-1} \neq \Lambda^N$ are not representations of $\mathrm{O}(2N)$. Instead, the direct sum of the two conjugate representations $\Lambda = (\Lambda^1, \dots, \Lambda^{N-1}, \Lambda^N)$ and $\bar{\Lambda} = (\Lambda^1, \dots, \Lambda^N, \Lambda^{N-1})$ of $\mathrm{SO}(2N)$ forms an irreducible representation of $\mathrm{O}(2N)$ [18]. Thus, for $\mathrm{SO}(2N)$

$$\chi_\Lambda(g) + \chi_{\bar{\Lambda}}(g) = 2\,\mathrm{Re}\,\chi_\Lambda(g) = \det\left[p_{\ell_i - N + j}(g) - p_{\ell_i - N - j}(g)\right]_{ij}. \tag{2.30}$$

To obtain the imaginary part, note that, whereas the first term in the numerator of (2.25d) is real, the second one changes sign for $\Lambda \to \bar{\Lambda}$ and is zero for $\Lambda = \bar{\Lambda}$ [18]. That is, the second term is the imaginary unit times the imaginary part of χ_Λ. It can be rewritten using the identity [157]

$$\det\left[\varepsilon_i^{N-j}(g) + \varepsilon_i^{-N+j}(g)\right]_{ij} = \frac{2}{\prod_k(\varepsilon_k(g) - \varepsilon_k(g)^{-1})} \det\left[\varepsilon_i^{N+1-j}(g) - \varepsilon_i^{-N-1+j}(g)\right]_{ij} \tag{2.31}$$

and $\operatorname{sign}(\ell_N) = \operatorname{sign}(\Lambda^N - \Lambda^{N-1})$ to

$$\mathrm{i}\,\mathrm{Im}\,\chi_\Lambda(g) = \frac{\operatorname{sign}(\ell_N)}{2} \prod_k(\varepsilon_k(g) - \varepsilon_k(g)^{-1}) \frac{\det\left[\varepsilon_i^{\ell_j}(g) - \varepsilon_i^{-\ell_j}(g)\right]_{ij}}{\det\left[\varepsilon_i^{N+1-j}(g) - \varepsilon_i^{-N-1+j}(g)\right]_{ij}}\,. \tag{2.32}$$

Comparing this with (2.25b) and (2.28b), one obtains the formula for the remaining representations of SO(2N), which depends on the sign of $\Lambda^{N-1} - \Lambda^N$. In summary, the results for SO(N) are

$$\chi_\Lambda(g) = \det\left[p_{\ell_i-N+j}(g) - p_{\ell_i-N-j}(g)\right]_{ij} \qquad \text{for SO}(2N+1), \tag{2.33a}$$

$$\chi_\Lambda(g) = \det\left[p_{\ell_i-N+j}(g) - p_{\ell_i-N-j}(g)\right]_{ij} \qquad \text{for SO}(2N) \text{ with } \Lambda^{N-1} = \Lambda^N\,, \tag{2.33b}$$

$$\begin{aligned}\chi_\Lambda(g) = {}& \frac{1}{2} \det\left[p_{\ell_i-N+j}(g) - p_{\ell_i-N-j}(g)\right]_{ij} + \\ & + \frac{\operatorname{sign}(\ell_N)}{4} \prod_k(\varepsilon_k(g) - \varepsilon_k(g)^{-1}) \det\left[p_{\ell_i-N+j-1}(g) + p_{\ell_i-N-j+1}(g)\right]_{ij} \\ & \qquad \text{for SO}(2N) \text{ with } \Lambda^{N-1} \neq \Lambda^N\,.\end{aligned} \tag{2.33c}$$

The Weyl character formulas thus obtained can be implemented on a computer with the help of a computer algebra system like Mathematica which provides routines for the series computation (2.27) needed to determine the p_i. This has been done in the package `DecomposeLGReps` presented in the following section.

VI.3 The package `DecomposeLGReps`

The Mathematica package `DecomposeLGReps` can be found on the webpage

http://einrichtungen.ph.tum.de/T30e/codes/DecomposeLGReps.

It contains implementations of the Weyl character formulas (2.25) as well as of the alternative forms shown in (2.28) and (2.33). For a detailed explanation of the functions and their options, the reader is referred to the package documentation shipped with the package. Here only the basic usage is briefly explained.

After loading the package with

```
Needs["DecomposeLGReps`"];
```

one has to specify the finite group that is to be embedded into a Lie group. This is done by providing a list containing one list for each irreducible representation of the finite group with the representation matrices of all group elements. Schematically this looks like

```
group = { { list of representation matrices of representation 1 },
          { list of representation matrices of representation 2 },
          ...
          { list of representation matrices of representation n } };
```

This list can, for example, be computed with the GAP interface package `Discrete` [158]. Alternatively, it is also possible just to specify representation matrices for one representative of each conjugacy class, see the package documentation for more information.

After this preparation, the finite group can be embedded into a Lie group using `embedinLG`,

```
embed = embedinLG[group, 12, "A"];
```

where the first argument is the list prepared before, the second argument specifies the representation that is used for the embedding following Section VI.1, and the last argument specifies the Lie group type.[5] If a reducible representation is to be embedded, a list of its irreducible constituents can be provided instead of a single integer as second argument. Hence, in the example the group is embedded into SU(N) $\sim A_{N-1} \sim$ `"A"` using the 12-th representation in the list `group`, where N is automatically chosen as the dimension of representation number 12. The representation chosen should, of course, be faithful; otherwise, the embedded group is not the desired one but a subgroup of it. An error is displayed if this is detected.

The last step is the actual computation of the decomposition of a Lie group representation specified by the Dynkin labels of its highest weight. This is done by the function `decomposeLGRep` in the following way:

```
decomposeLGRep[{a1, a2,..., aN}, embed]
```

The first argument is a list with the Dynkin labels and the second argument is the output of `embedinLG`. The Lie group type is also taken from there in order to avoid a mismatch between the Lie group of the embedding and the Lie group for which the branching rule is to be computed. The output of `decomposeLGRep` is a list containing the multiplicities of representations of the finite group in the decomposition of the Lie group representation with the Dynkin labels `(a1, a2, ..., aN)`. The order of the multiplicities in the output is identical to the one of representations 1 to n specified earlier in the variable `group`.

As an example, let `a4Matrices` contain the representation matrices of the tetrahedral group A_4 in the form shown above and in the order ($\mathbf{1}$, $\mathbf{1}'$, $\mathbf{1}''$, $\mathbf{3}$) where the notation of [73] is used, see also Section A.1.1. The tetrahedral group can be embedded into SU(3) using the faithful triplet representation $\mathbf{3}$.[6] This is done by the command

```
embedA4 = embedinLG[a4Matrices, 4, "A"];
```

To avoid confusion with the group name A_4, let us again remark that the 4 stands for the fourth representation in the list `a4Matrices`, which is assumed to be ordered as ($\mathbf{1}$, $\mathbf{1}'$, $\mathbf{1}''$, $\mathbf{3}$), and `"A"` for the Lie algebra of SU(N). The decomposition of the fundamental representation of SU(3) can then be computed by

```
decomposeLGRep[{1, 0}, embedA4]
```

which yields

5 Possible types are `"A"` for SU(N) and U(N), `"B"` for SO($2N+1$), `"C"` for USp($2N$) and `"D"` for SO($2N$).
6 In fact, it is a subgroup of SO(3), see the following section.

```
{0, 0, 0, 1}
```

i.e. the fundamental of SU(3) contains once the **3** of A_4 and no other representation. This just shows that the embedding worked out correctly. One can now compute more branching rules, e.g.

```
decomposeLGRep[{2, 0}, embedA4]  -> {1, 1, 1, 1}
decomposeLGRep[{1, 1}, embedA4]  -> {0, 1, 1, 2}
decomposeLGRep[{23, 15}, embedA4] -> {640, 640, 640, 1920}
```

For more examples and explanations of all options, see the package manual included in the download.

Note that the package was checked for correctness against results for branching rules from the literature. Indeed, all branching rules presented by Luhn and Ramond [111] and Luhn [151] were reproduced successfully. For the decompositions $SO(3) \to A_4$, $SO(3) \to S_4$ and $SU(3) \to \Delta(27)$, this consistency check can easily be repeated by specialising the general formulas shown in the following section to the representations of smallest dimension.

VI.4 Examples for small finite groups

Using the MATHEMATICA package `DecomposeLGReps` presented in the previous section, one can derive general results for branching rules to some well-known finite groups. This can be done by applying the character formulas (2.25), which allow for generic non-negative integer inputs for the Dynkin labels of the representations which are to be decomposed. In all cases not only the exact functions determining the branching are interesting. In addition, the insight gained on the structure, i.e. on which representations are contained within which (congruence) class [159] of representations of the continuous group, is very helpful for model building. The examples chosen are A_4, T', S_4, A_5, $\Delta(27)$ and $\Delta(54)$. Further information on all these groups can be found in [57] although the notation used here is partly different. References to the notations used are given for each case individually below. In many cases, the results are actually independent of the specific naming convention, e.g. in A_4 the results do not depend on which representation is called $\mathbf{1}'$ and which one $\mathbf{1}''$.

The following abbreviations are used for functions that occur several times:

$$f(n,m) := (1+n)\,(1+3m+n)\,(2+3m+2n)\,, \tag{4.1a}$$

$$p^+(n) := \cos\left(\frac{n\,\pi}{3}\right) + \frac{1}{\sqrt{3}}\sin\left(\frac{n\,\pi}{3}\right) = \begin{cases} 1, & n \equiv 0,1 \pmod 6, \\ 0, & n \equiv 2,5 \pmod 6, \\ -1, & n \equiv 3,4 \pmod 6, \end{cases} \tag{4.1b}$$

$$p^-(n) := \cos\left(\frac{n\,\pi}{3}\right) - \frac{1}{\sqrt{3}}\sin\left(\frac{n\,\pi}{3}\right) = \begin{cases} 1, & n \equiv 0,5 \pmod 6, \\ 0, & n \equiv 1,4 \pmod 6, \\ -1, & n \equiv 2,3 \pmod 6, \end{cases} \tag{4.1c}$$

$$q(n) := \cos\left(\frac{4\,n\,\pi}{3}\right) + \frac{1}{\sqrt{3}}\sin\left(\frac{4\,n\,\pi}{3}\right) = \begin{cases} 1, & n \equiv 0 \pmod 3, \\ 0, & n \equiv 2 \pmod 3, \\ -1, & n \equiv 1 \pmod 3. \end{cases} \tag{4.1d}$$

Λ	$\to$	$\mathbf{1}$	$\mathbf{1}'$	$\mathbf{1}''$	$\mathbf{3}$
$(12\,n)$	$\to$	$n+1$	n	n	$3n$
$(12\,n+2)$	$\to$	n	n	n	$3n+1$
$(12\,n+4)$	$\to$	n	$n+1$	$n+1$	$3n+1$
$(12\,n+6)$	$\to$	$n+1$	n	n	$3n+2$
$(12\,n+8)$	$\to$	$n+1$	$n+1$	$n+1$	$3n+2$
$(12\,n+10)$	$\to$	n	$n+1$	$n+1$	$3(n+1)$

Table VI.2: Branching rules for the embedding $\mathrm{A}_4 \hookrightarrow \mathrm{SO}(3)$ using the triplet representation of A_4. SO(3) representations are denoted by the Dynkin labels Λ of their highest weights. Only proper SO(3) representations are considered, i.e. Λ is even, see Section VI.1. For the conventions used, see Section A.1.1.

VI.4.1 A_4

The tetrahedral group A_4 of the example model by Altarelli and Feruglio [9, 10] is a subgroup of SO(3); the embedding proceeds via the only three-dimensional representation **3**. For the conventions used, see Section A.1.1.

The decomposition formulas are most easily displayed if the SO(3) representations are split into five classes with Dynkin labels taking the forms $(12\,n+2m)$ for $m = 0,\dots,5$.[7] The resulting multiplicities are displayed in Table VI.2. Setting n to zero one obtains the branching rules for SO(3) representations up to dimension 11. They are identical to the decomposition rules derived by Luhn and Ramond [111].

The smallest SO(3) representation containing a trivial A_4 singlet is the representation with Dynkin label (6), which using its dimension as label can also be denoted **7**.

VI.4.2 T′

The group T′ of the second example model used in Chapter V is not a subgroup of SO(3) but can be embedded into SU(2) using its representation $\mathbf{2}_0$. The naming conventions are summarised in Section A.1.2.

Splitting the SU(2) representations into the two classes of vector $(2\,n)$ and spinor $(2\,n+1)$ representations, the decomposition yields

$$\begin{aligned}(2\,n) \to{}& \frac{1}{12}\left[2n+(-1)^n\,(8\,p^-(n)+9)+1\right]\times\mathbf{1}_0\\ &\oplus\frac{1}{12}\left[2n+(-1)^n\,(-4\,p^-(n)+9)+1\right]\times(\mathbf{1}_1\oplus\mathbf{1}_2)\\ &\oplus\frac{1}{4}\left(2n+(-1)^{n+1}+1\right)\times\mathbf{3}\,,\end{aligned} \tag{4.2a}$$

$$\begin{aligned}(2\,n+1) \to{}& \frac{1}{3}\left(n+2\,(-1)^n\,p^+(n)+1\right)\times\mathbf{2}_0\\ &\oplus\frac{1}{3}\left(n+(-1)^{1+n}\,p^+(n)+1\right)\times(\mathbf{2}_1\oplus\mathbf{2}_2)\,.\end{aligned} \tag{4.2b}$$

In fact, the decomposition for vector representations is exactly the same as the one for $\mathrm{A}_4 \hookrightarrow \mathrm{SO}(3)$ shown in Table VI.2 with the change of notation $\mathbf{1}\to\mathbf{1}_0$, $\mathbf{1}'\to\mathbf{1}_1$ and $\mathbf{1}''\to\mathbf{1}_2$.

7 Note that, since A_4 is embedded into SO(3) (in contrast to SU(2)), only non-spinorial, i.e. genuine, representations of SO(3) are considered, see the discussion at the end of Section VI.1.

Λ	$\to$	$\mathbf{2}_0$	$\mathbf{2}_1$	$\mathbf{2}_2$
$(12n+1)$	$\to$	$2n+1$	$2n$	$2n$
$(12n+3)$	$\to$	$2n$	$2n+1$	$2n+1$
$(12n+5)$	$\to$	$2n+1$	$2n+1$	$2n+1$
$(12n+7)$	$\to$	$2(n+1)$	$2n+1$	$2n+1$
$(12n+9)$	$\to$	$2n+1$	$2(n+1)$	$2(n+1)$
$(12n+11)$	$\to$	$2(n+1)$	$2(n+1)$	$2(n+1)$

Table VI.3: Branching rules for the embedding $\mathrm{T}' \hookrightarrow \mathrm{SU}(2)$ using the doublet $\mathbf{2}_0$ of T'. $\mathrm{SU}(2)$ representations are denoted by the Dynkin labels Λ of their highest weights. Only $\mathrm{SU}(2)$ spinor representations are considered because the branching rules for non-spinorial representations are the same as for A_4 shown in Table VI.2. For the T' notation used, see Section A.1.2.

Λ	$\to$	$\mathbf{1}$	$\mathbf{1}'$	$\mathbf{2}$	$\mathbf{3}$	$\mathbf{3}'$
$(12n)$	$\to$	$\frac{2n+(-1)^n+3}{4}$	$\frac{2n+(-1)^{n+1}+1}{4}$	n	$\frac{6n+(-1)^n-1}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$
$(12n+2)$	$\to$	$\frac{2n+(-1)^n-1}{4}$	$\frac{2n+(-1)^{n+1}+1}{4}$	n	$\frac{6n+(-1)^n+3}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$
$(12n+4)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{2n+(-1)^n-1}{4}$	$n+1$	$\frac{6n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^n+3}{4}$
$(12n+6)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{2n+(-1)^n+3}{4}$	n	$\frac{6n+(-1)^{n+1}+5}{4}$	$\frac{6n+(-1)^n+3}{4}$
$(12n+8)$	$\to$	$\frac{2n+(-1)^n+3}{4}$	$\frac{2n+(-1)^{n+1}+1}{4}$	$n+1$	$\frac{6n+(-1)^n+3}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$
$(12n+10)$	$\to$	$\frac{2n+(-1)^n-1}{4}$	$\frac{2n+(-1)^{n+1}+1}{4}$	$n+1$	$\frac{6n+(-1)^n+7}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$

Table VI.4: Branching rules for the embedding $\mathrm{S}_4 \hookrightarrow \mathrm{SO}(3)$ using the triplet representation $\mathbf{3}'$ of S_4. $\mathrm{SO}(3)$ representations are denoted by the Dynkin labels Λ of their highest weights. For the conventions used, see [73].

For spinor representations the formulas above can be recast as shown in Table VI.3. This shows that the doublet representations of T', which are not representations of A_4, are 'spinor' representations and can only be obtained from spinor representations of $\mathrm{SU}(2)$. In particular, spinor representations of $\mathrm{SU}(2)$ cannot be used to break $\mathrm{SU}(2)$ to T' because they do not contain trivial T' singlets.

VI.4.3 S_4

The same classes as for A_4 can be used for S_4, which is also a subgroup of $\mathrm{SO}(3)$. It was used early on in flavour model building [160] and is still popular because it, too, can lead to tri-bi-maximal mixing. The embedding proceeds via representation $\mathbf{3}'$. The other three-dimensional representation $\mathbf{3}$ would lead to an embedding into $\mathrm{O}(3)$ because not all determinants of its representation matrices are $+1$. Here, the notation from [73] is used.

The results are shown in Table VI.4. The first trivial singlet occurs for the representation with Dynkin label (8), which can also be called $\mathbf{9}$. Again, the results for $\mathrm{SO}(3)$ representations up to dimension 11 are the same as already presented in [111].

VI.4.4 A_5

The last missing subgroup of SO(3) with an irreducible triplet representation is the icosahedral group, which is isomorphic to the alternating group on five letters A_5. It is the largest non-abelian subgroup of SO(3) with such a representation. A_5 can lead to golden ratio mixing when applied to neutrino model building [84] and is, as a simple group, intrinsically anomaly safe, see Chapter IV. For recent model building approaches using this group see [123, 124]. Again the notation from [73] is used.

The Dynkin labels of SO(3) are split into the classes $(30\,n + 2\,m)$ for $m = 0, \ldots, 14$. The results are shown in Table VI.5. They show that the first singlet is contained in representation **13** with Dynkin label (12).

VI.4.5 $\Delta(27)$

The group $\Delta(27)$ can be embedded into SU(3) using its triplet representation **3**. It is part of the infinite series of $\Delta(3 \cdot n^2)$ subgroups of SU(3). $\Delta(27)$ is well known in model building for the so-called geometrical spontaneous CP violation [4, 15, 17, 161], see also Section VII.10. The conventions are as shown in Section A.1.3.

The decomposition properties of representations of SU(3) labelled by their Dynkin labels (a_1, a_2) can be most easily described by splitting them into three different classes. Their Dynkin labels take the forms $(n, n + 3m)$, $(n, n + 3m + 1)$ and $(n, n + 3m + 2)$, where n and m are integers. These three classes are related to the triality classes of SU(3) [159]. $(n, n + 3m)$ is in class 0, i.e. the real class or the class of the adjoint representation, $(n, n + 3m + 1)$ in class 2, i.e. the class of the anti-fundamental representation, and $(n, n + 3m + 2)$ in class 1, i.e. of the fundamental representation. The resulting decomposition rules for the three classes are

$$\begin{aligned}(n, n+3m) \to \frac{1}{18}\,&\left(f(n,m) + 16\,(-1)^n p^+(n)\right) \times \mathbf{1}_0 \\ &\oplus \frac{1}{18}\,\left(f(n,m) - 2\,q(n)\right) \times \bigoplus_{i=1}^{8} \mathbf{1}_i\,,\end{aligned} \tag{4.3a}$$

$$(n, n+3m+1) \to \frac{1}{6}\,(1+n)\,(2+3m+n)\,(3+3m+2n) \times \overline{\mathbf{3}}\,, \tag{4.3b}$$

$$(n, n+3m+2) \to \frac{1}{6}\,(1+n)\,(3+3m+n)\,(4+3m+2n) \times \mathbf{3}\,. \tag{4.3c}$$

Hence, all real representations of SU(3) branch to a direct sum of trivial singlets and full sets of non-trivial $\Delta(27)$ singlets. Moreover, the class of the fundamental SU(3) representation yields only triplets and, accordingly, the class of the anti-fundamental only anti-triplets of $\Delta(27)$. The group $\Delta(27)$ is thus very much aligned with the structure of SU(3), making it, for example, impossible to obtain a CP breaking representation content via spontaneous breaking, see Section VII.9.3 below.

Specialising to SU(3) representations up to dimension 27, the results coincide with the ones presented in [111, 151].

VI.4.6 $\Delta(54)$

As a second example of an SU(3) subgroup, consider $\Delta(54)$. $\Delta(54)$ is part of the $\Delta(6 \cdot n^2)$ series of SU(3) subgroups. It turns out that, due to the additional continuous symmetries, $\Delta(54)$ is the realised discrete symmetry group of the $\Delta(27)$ Higgs potentials leading to geometrical

Λ	$\to$	**1**	**3**	**3′**	**4**	**5**
$(30\,n)$	$\to$	$\frac{2n+(-1)^n+3}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$	$2n$	$\frac{10n+(-1)^n-1}{4}$
$(30\,n+2)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^n+3}{4}$	$\frac{6n+(-1)^n-1}{4}$	$2n$	$\frac{10n+(-1)^{n+1}+1}{4}$
$(30\,n+4)$	$\to$	$\frac{2n+(-1)^n-1}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$	$2n$	$\frac{10n+(-1)^n+3}{4}$
$(30\,n+6)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^n-1}{4}$	$\frac{6n+(-1)^n+3}{4}$	$2n+1$	$\frac{10n+(-1)^{n+1}+1}{4}$
$(30\,n+8)$	$\to$	$\frac{2n+(-1)^n-1}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$	$2n+1$	$\frac{10n+(-1)^n+3}{4}$
$(30\,n+10)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^n+3}{4}$	$\frac{6n+(-1)^n+3}{4}$	$2n$	$\frac{10n+(-1)^{n+1}+5}{4}$
$(30\,n+12)$	$\to$	$\frac{2n+(-1)^n+3}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$	$2n+1$	$\frac{10n+(-1)^n+3}{4}$
$(30\,n+14)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^n+3}{4}$	$\frac{6n+(-1)^n+3}{4}$	$2n+1$	$\frac{10n+(-1)^{n+1}+5}{4}$
$(30\,n+16)$	$\to$	$\frac{2n+(-1)^n-1}{4}$	$\frac{6n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$	$2n+1$	$\frac{10n+(-1)^n+7}{4}$
$(30\,n+18)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^n+3}{4}$	$\frac{6n+(-1)^n+3}{4}$	$2(n+1)$	$\frac{10n+(-1)^{n+1}+5}{4}$
$(30\,n+20)$	$\to$	$\frac{2n+(-1)^n+3}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$	$2n+1$	$\frac{10n+(-1)^n+7}{4}$
$(30\,n+22)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^n+7}{4}$	$\frac{6n+(-1)^n+3}{4}$	$2n+1$	$\frac{10n+(-1)^{n+1}+9}{4}$
$(30\,n+24)$	$\to$	$\frac{2n+(-1)^n+3}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$	$2(n+1)$	$\frac{10n+(-1)^n+7}{4}$
$(30\,n+26)$	$\to$	$\frac{2n+(-1)^{n+1}+1}{4}$	$\frac{6n+(-1)^n+3}{4}$	$\frac{6n+(-1)^n+7}{4}$	$2(n+1)$	$\frac{10n+(-1)^{n+1}+9}{4}$
$(30\,n+28)$	$\to$	$\frac{2n+(-1)^n-1}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$	$\frac{6n+(-1)^{n+1}+5}{4}$	$2(n+1)$	$\frac{10n+(-1)^n+11}{4}$

Table VI.5: Branching rules for the embedding $A_5 \hookrightarrow SO(3)$ using the triplet representation **3** of A_5. $SO(3)$ representations are denoted by the Dynkin labels Λ of their highest weights. For the conventions used, see [73].

CP violation [161–163]. The group is embedded into SU(3) using its three-dimensional representation $\mathbf{3}_2$. Note that there is a second three-dimensional representation $\mathbf{3}_1$, whose representation matrices do not all have determinant +1. Hence, this representation would embed $\Delta(54)$ into U(3) instead of SU(3). The conventions are shown in Section A.1.4.

The representations of SU(3) are again divided into the three classes described for $\Delta(27)$ above. The resulting decomposition rules for the three classes are

$$\begin{aligned}(n,\, n+3m) \to \frac{1}{72}\,&\big[9\,(-1)^n\,\left((-1)^m\,(3m+n+1)+n+1\right)\\ &\quad+(3m+2n+2)\,\left(2\,(n+1)\,(3m+n+1)+9(-1)^m\right)\\ &\quad+32\,(-1)^n\,p^+(n)\big]\times\mathbf{1}_0\\ \oplus\frac{1}{72}\,&\big[-9\,(-1)^n\,\left((-1)^m\,(3m+n+1)+n+1\right)\\ &\quad+(3m+2n+2)\,\left(2\,(n+1)\,(3m+n+1)-9(-1)^m\right)\\ &\quad+32\,(-1)^n\,p^+(n)\big]\times\mathbf{1}_1\\ \oplus\frac{1}{18}\,&\big[f(n,m)-2\,q(n)\big]\times\bigoplus_{i=1}^{4}\mathbf{2}_i\,,\end{aligned} \tag{4.4a}$$

$$\begin{aligned}(n,\, n+3m+1) \to \frac{1}{24}\,&\big[(3m+2n+3)\,\left(2\,(n+1)\,(3m+n+2)+3\,(-1)^m\right)\\ &\quad+3\left((-1)^{m+1}\,(n+1)+3m+n+2\right)(-1)^{m+n}\big]\times\overline{\mathbf{3}}_2\\ \oplus\frac{1}{24}\,&\big[3\,(-1)^m\,\left((-1)^{n+1}\,(3m+n+2)-3m-2n-3\right)\\ &\quad+(n+1)\,\left(2\,(3m+n+2)\,(3m+2n+3)+3\,(-1)^n\right)\big]\times\overline{\mathbf{3}}_1\,,\end{aligned} \tag{4.4b}$$

$$\begin{aligned}(n,\, n+3m+2) \to \frac{1}{24}\,&\big[(3m+2n+4)\,\left(2\,(n+1)\,(3m+n+3)-3\,(-1)^m\right)\\ &\quad-3\,\left((-1)^m\,(n+1)+3m+n+3\right)(-1)^{n+m}\big]\times\mathbf{3}_2\\ \oplus\frac{1}{24}\,&\big[(3m+2n+4)\,\left(2\,(n+1)\,(3m+n+3)+3\,(-1)^m\right)\\ &\quad+3\,\left((-1)^m\,(n+1)+3m+n+3\right)(-1)^{n+m}\big]\times\mathbf{3}_1\,.\end{aligned} \tag{4.4c}$$

Although the formulas are considerably more complicated than the ones for $\Delta(27)$, it is easy to see that $\Delta(54)$ is also closely aligned to the structure of SU(3). Again, the real class of SU(3) representations yields trivial singlets and complete sets of doublets (which contain the non-trivial singlets of $\Delta(27)$), whereas the fundamental and anti-fundamental classes contain triplets and anti-triplets, respectively.

The smallest representation of SU(3) containing a trivial $\Delta(54)$ singlet is the **27**, which, in fact, contains three trivial $\Delta(54)$ singlets. This result is in agreement with [151].

VI.5 Conclusion of the chapter

It was shown how to obtain the branching rules for the breaking of compact classical Lie groups to finite subgroups thereof using the character scalar product. This information is important when building models where discrete non-abelian symmetries are obtained by spontaneously breaking a continuous symmetry group. The embedding of a finite subgroup into a Lie group is specified by an explicit matrix representation of the finite group, which

is then viewed as a restriction of the fundamental representation of the Lie group to the finite group.

To compute the characters of group elements for arbitrary irreducible Lie group representations, the Weyl character formula for Lie algebra characters was reviewed and its applicability to the problem in question established. Two different, but of course equivalent, forms of the Weyl character formula in terms of the eigenvalues of the representation matrices specifying the embedding were presented. These formulas are implemented in form of the MATHEMATICA package `DecomposeLGReps` that can be found online.[8] It can be used to compute branching rules for arbitrary non-abelian finite subgroups of the compact classical Lie groups $\mathrm{U}(N)$, $\mathrm{SU}(N)$, $\mathrm{SO}(N)$ and $\mathrm{USp}(2N)$, limited only by computational power. The usage of this package was briefly outlined; more information can be found in the manual that is included in the download.

As an application of the package, general branching rules as functions of the Dynkin labels for various small finite groups were derived. The results provide insights into the breaking patterns available for these finite groups. For example, it was shown explicitly that the doublet representations of T′ only arise as remnants of $\mathrm{SU}(2)$ spinor, in contrast to vector, representations. Another result is that breaking $\mathrm{SU}(3)$ to $\Delta(27)$ one cannot obtain a single non-trivial singlet representation but only complete sets of non-trivial singlets. This result is important for the discussion of spontaneous CP violation in Chapter VII. In general, such information is very useful for (flavour) model building with spontaneously broken continuous symmetries because certain structures of the potential can be envisaged directly from the branching rules of the symmetry.

8 http://einrichtungen.ph.tum.de/T30e/codes/DecomposeLGReps

VII Generalised CP

A crucial part of the flavour puzzle of the Standard Model described in Chapter III is the existence of a non-trivial CP violating phase δ_{CP}. Giving a reason for CP violation and predicting its size from some underlying principle is therefore an important aim of models of physics beyond the SM. As for the mixing structure and the mass hierarchy, one might be inclined to tackle this problem using additional symmetries, i.e. flavour symmetries, which for the reasons outlined in Chapter III might be chosen to be non-abelian and discrete. It is hence essential to understand how to generalise the CP transformation of the SM to such models with additional discrete flavour symmetries. At first glance this task seems simple; however, a difficult interplay of mathematical and physical constraints renders it highly non-trivial. This generalisation of the CP transformations of Quantum electrodynamics (QED) and the Standard Model to theories with (non-abelian) discrete symmetries shall thus be discussed here in great detail.

As starting point, parity transformation, time reversal and charge conjugation are discussed as symmetries of QED in Section VII.1.1. The only difficulty one faces here is to determine the transformation behaviour of spinor fields, i.e. to find transformations that are consistent with the structure of the Lorentz or, rather, Poincaré group. However, this is not the focus of the present text; detailed discussions of this issue can be found in any quantum field theory textbook, e.g. [29]. Starting from the definition in the context of QED, the inversion symmetries are then discussed in the context of the Standard Model in Section VII.1.2. As is immediately clear from the field content, charge conjugation and parity cannot be discussed individually but only in the form of a combined CP transformation. However, even this transformation is not a symmetry of the SM, which makes it difficult to uniquely define it. This is further discussed in Section VII.2, where it is explained why only the additional composition with time reversal, i.e. CPT, is a uniquely defined transformation and symmetry of a quantum field theory.

Albeit it is explicitly broken, one can, of course, still define a CP transformation for the Standard Model, and it is important to understand how to generalise this to models of physics beyond the Standard Model. For example, in order to give an explanation of the CP properties of the SM in terms of spontaneous breaking of CP in a more fundamental theory, one must first define and understand a consistent CP transformation in this theory. In particular, the relation of CP symmetries to the various other symmetry groups of a model is important. For gauge symmetries, this was discussed by Grimus and Rebelo [14]; their results are briefly reviewed in Section VII.3.1. Holthausen, Lindner and Schmidt [15]

* Some of the results presented in this chapter have already been communicated in [3, 4].

and Feruglio, Hagedorn and Ziegler [16] partly transferred these results to models with discrete symmetries, and their findings are reviewed in Section VII.3.2.

However, in Section VII.4, it is argued that their conditions are, although under some assumptions sufficient for purely mathematical consistency, not sufficient to obtain physical CP transformations, i.e. transformations which should be considered extensions of the Standard Model CP transformation. This leads us to refine the conditions on CP transformations in the presence of discrete symmetries. As these revised conditions are non-trivial, it turns out that not all groups allow for CP transformations in generic settings; a statement that is clarified carefully below. Moreover, only some groups allow the usual canonical CP transformation to be implemented. These groups, which are classified as type II A groups below, have a basis in which all Clebsch–Gordan coefficients are real. This latter statement builds on the equivalence of the existence of such a basis and the existence of a certain type of automorphism for a given group that was first proved by Bickerstaff and Damhus [164]. Their statement is thus reviewed and connected to our new results in Section VII.5. Furthermore, the so-called twisted Frobenius–Schur indicator is introduced in Section VII.6 as a means to test whether a given group has such an automorphism or not, and, in the latter case, whether it still allows for a consistent CP transformation or whether one cannot define CP for this group.

It is then discussed in Section VII.8 how these generalised CP transformations constrain the couplings of a given model. This is illustrated in Section VII.9 with examples for the three different types of groups, i.e. groups with the canonical CP transformation (type II A), groups with a different CP transformation (type II B) and groups without any CP transformation in generic settings (type I). Furthermore, a toy model is presented which proves that it is possible to spontaneously break a type II group to a type I group in such a way that CP is violated with calculable phases, i.e. phases that do not depend on couplings but only on the group theory of the model.

A famous model where CP is spontaneously violated by a vacuum expectation value with phases which are independent of the couplings was devised by Branco, Gerard and Grimus [17]. Section VII.10 reviews this so-called geometrical CP violation and corrects a frequent misunderstanding of this effect.

Although the approach of flavour symmetries is usually focussed on the flavour and associated weak CP problem, one might hope that the acquired knowledge could as well be used to find new possibilities for a solution to the strong CP problem. Unfortunately, no genuinely different solutions can be obtained, as discussed in Section VII.11.

For a final explanation of the (weak) CP violation in the Standard Model, i.e. the question why δ_{CP} has the measured value, it is desirable to break CP spontaneously, if possible with phases that are independent of couplings. New aspects of spontaneous symmetry breaking arising from the generalisation of CP to discrete groups are presented in Section VII.12.

Subsequently, in Section VII.13, the criteria by Grimus and Rebelo [14] on CP transformations for continuous groups are examined again for additional conditions that could be imposed on physical CP transformations of discrete symmetries.

Finally, after concluding, some comments on various claims in the literature are compiled.

VII.1 Inversion symmetries in QED and the Standard Model

For the discussion of generalised CP transformations, it is necessary to understand the general idea of these inversion symmetries. It is thus instructive first to discuss them in the

context of Quantum Electrodynamics (QED), i.e. of a $\mathrm{U}(1)$ gauge theory with one charged fermion described by a Dirac spinor. This is, on the one hand, arguably the simplest theory with meaningful parity, time reversal and charge conjugation transformations, and, on the other hand, it allows by comparison with classical electrodynamics an intuitive approach to the subject.

In contrast to that, the definition of inversion symmetries for the Standard Model is more involved. As the SM and its extensions are the theories of interest, the inversion symmetries of the SM are discussed below in order to lay the foundation for their subsequent generalisation.

The transformation formulas collected in this section are taken from [29], whose notation and conventions are also used.

VII.1.1 Inversion symmetries in QED

Parity

Parity P is defined to be the inversion of spatial coordinates. Thus, it acts on a space-time coordinate x^μ as

$$x^\mu = (x^0, x^i) \overset{P}{\longmapsto} x^\mu_P := (x^0, -x^i)\,. \tag{1.1}$$

It is the transformation that connects proper orthochronous Lorentz transformations, i.e. transformations of $\mathrm{SO}(1,3)^+$, to improper orthochronous Lorentz transformations. In analogy to its action on spatial coordinates, parity reverses three-momentum and helicity, while energy and angular momentum are invariant.

When implementing this transformation on a Hilbert space as an operator $\boldsymbol{P}$, the operator must be linear in order to be able to obtain a positive spectrum for a parity invariant theory [165].[1]

Parity relates the representation (j, j') of $\mathrm{SO}(1,3)^+$ to the representation (j', j) [166], i.e. it changes the chirality (handedness) of a field. For a scalar field this is, of course, no concern and parity acts as

$$\boldsymbol{P}\,\boldsymbol{\Phi}(x)\,\boldsymbol{P}^{-1} = \mathrm{e}^{\mathrm{i}\,\gamma}\;\boldsymbol{\Phi}(x_P)\,, \tag{1.2}$$

with a free phase γ, which just parametrises the quantum mechanical freedom to re-phase a field operator. This freedom is captured by a phase called γ throughout this section without further mention.

Note that due to the change $x \mapsto x_P$ of the argument of the field, a Lagrangian is not invariant under parity but transforms in the parity conserving case as $\mathcal{L}(x) \mapsto \mathcal{L}(x_P)$. Due to the integration over all space-time coordinates, the respective action is, however, invariant, i.e. parity is not a symmetry of the Lagrangian but of the action.

For spinor fields the change of chirality becomes an issue because a Weyl spinor λ_α in $(1/2, 0)$ would have to be mapped to a spinor in the $(0, 1/2)$ representation. If the particle is charged under a symmetry like $\mathrm{U}(1)_{\mathrm{em}}$, there is, a priori, no such state with the same charge to which λ_α could be mapped. This issue does not arise in QED because the electron is described by a Dirac spinor, i.e. it transforms in the representation $(1/2, 0) \oplus (0, 1/2)$, and parity can be implemented by

$$\boldsymbol{P}\,\boldsymbol{\Psi}(x)\,\boldsymbol{P}^{-1} = \mathrm{e}^{\mathrm{i}\,\gamma}\;\gamma^0\,\boldsymbol{\Psi}(x_P)\,. \tag{1.3}$$

1 For Wigner's representation theorem and linear and anti-linear operators, see Section A.3.

The transformation of the electromagnetic field can then be inferred from its coupling to the electron insisting that this term be invariant. This leads to

$$\boldsymbol{P}\,\boldsymbol{A}^{\mu}(x)\,\boldsymbol{P}^{-1} = \varepsilon(\mu)\,\boldsymbol{A}^{\mu}(x_P)\,, \tag{1.4}$$

where the function

$$\varepsilon(\mu) := \begin{cases} 1\,, & \mu = 0\,, \\ -1\,, & \text{otherwise}, \end{cases} \tag{1.5}$$

is introduced.

Time reversal

As explained below, the name time reversal is actually a slight misnomer. Moreover, there are several transformations that are called time reversal in the literature [167, 168]. One of them is the analogous transformation to parity in the sense that it is the Lorentz transformation sending the proper orthochronous subgroup to the proper anti-chronous coset, i.e. the transformation that acts on the spatial coordinates as

$$x^{\mu} = (x^0, x^i) \overset{T}{\longmapsto} x^{\mu}_T := (-x^0, x^i) \tag{1.6}$$

and in the same way on any other four-vector, e.g. on the momentum. Since this also multiplies the energy as zero-th component p^0 of the momentum with -1, one cannot implement this as a symmetry in a theory with a stable ground state, cf. e.g. [29, 165].

One solution is a time reversal as introduced by Schwinger [169], cf. also [167, 168], which in addition to the transformation described above acts as a charge conjugation. This is not discussed any further here.

Most often, however, a transformation defined by Wigner [170] is called time reversal, although a better name would perhaps be motion reversal, cf. [168]. Its classical analogue acts like running a film backwards: the properties of particles are unchanged but particles move in the opposite direction with time, ending up at their starting point. This transformation is also usually meant with T when talking about the CPT theorem, see below, and it is this operation that the term time reversal refers to in the following.

The Wigner time reversal acts on spatial coordinates as shown in (1.6) but, in contrast to the Schwinger time reversal, does not invert the charges of any field. In order to arrive at a spectrum bounded below, the corresponding Hilbert space operator $\boldsymbol{T}$ must be chosen anti-linear. In the S-matrix picture, time reversal inverts the direction of motion of every incoming and outgoing particle, reverses their spins and exchanges incoming and outgoing particles [165]. Its action on a scalar field operator is thus

$$\boldsymbol{T}\,\boldsymbol{\Phi}(x)\,\boldsymbol{T}^{-1} = \mathrm{e}^{\mathrm{i}\,\gamma}\;\boldsymbol{\Phi}(x_T)\,. \tag{1.7}$$

As there is only an inversion of the direction of motion, there is, of course no issue with missing states as for parity, i.e. time reversal can also be implemented in theories with only a single Weyl fermion. For the discussion of QED, the transformation

$$\boldsymbol{T}\,\boldsymbol{\Psi}(x)\,\boldsymbol{T}^{-1} = \mathrm{e}^{\mathrm{i}\,\gamma}\,(\mathrm{i}\;\gamma^1\,\gamma^3)\;\boldsymbol{\Psi}(x_T) \tag{1.8}$$

of a Dirac spinor is sufficient, though. Using again the coupling of the electromagnetic gauge boson to the fermion current and demanding invariance of this term, one obtains the transformation behaviour

$$\boldsymbol{T}\,\boldsymbol{A}^{\mu}(x)\,\boldsymbol{T}^{-1} = \varepsilon(\mu)\,\boldsymbol{A}^{\mu}(x_T) \tag{1.9}$$

of the gauge boson under time reversal.

Note that, in complete analogy to parity, a Lagrangian is usually not invariant under time reversal even if its space-time integral, i.e. its action, is, due to the change of the argument of fields. Invariance of the action is, of course, sufficient for time reversal to be a symmetry of the theory in question.

Charge conjugation

The action of charge conjugation is a priori not related to the Lorentz structure of a theory, although it can, in fact, be related to it, cf. [168]. In QED the definition of charge conjugation seems clear: it replaces an electron with a positron and vice versa without changing anything else. Note that this operation can only be implemented as a symmetry acting on a Weyl spinor if there is another Weyl spinor in the complex conjugate representation, i.e. with the opposite charge. This is the case because, otherwise, the two Hilbert spaces of original and charge conjugated fields could not be identified [29]. The condition is by construction fulfilled for Dirac spinors and their transformation behaviour is[2]

$$\boldsymbol{C}\,\boldsymbol{\Psi}(x)\,\boldsymbol{C}^{-1} = \mathrm{e}^{\mathrm{i}\,\gamma}\,(\mathrm{i}\,\gamma^0\,\gamma^2)\,\overline{\boldsymbol{\Psi}}^{T}(x) =: \mathrm{e}^{\mathrm{i}\,\gamma}\;\boldsymbol{\Psi}^{c}(x)\,, \tag{1.10}$$

where $\overline{\boldsymbol{\Psi}} := \boldsymbol{\Psi}^{\dagger}\,\gamma^0$ and where $\boldsymbol{C}$ is a linear, unitary operator. Analogously, the transformation of a scalar is

$$\boldsymbol{C}\,\boldsymbol{\Phi}(x)\,\boldsymbol{C}^{-1} = \mathrm{e}^{\mathrm{i}\,\gamma}\;\boldsymbol{\Phi}^{\dagger}(x)\,. \tag{1.11}$$

By the same arguments as above, the gauge boson transforms as

$$\boldsymbol{C}\,\boldsymbol{A}^{\mu}(x)\,\boldsymbol{C}^{-1} = -\boldsymbol{A}^{\mu}(x)\,. \tag{1.12}$$

VII.1.2 Inversion symmetries in the Standard Model

The extension of the concepts of parity, time reversal and charge conjugation from QED to the Standard Model might seem straightforward. However, the Standard Model is a completely different type of theory because it is chiral and thus not invariant under parity or charge conjugation. This is clear immediately from its matter content, see Table III.1, as there is, for example, no parity or charge conjugation partner for the left-handed $\mathrm{SU}(2)_{\mathrm{L}}$ lepton doublet. Thus, parity and charge conjugation are broken in the Standard Model by the field or representation content. In fact, it is impossible consistently to define these transformations. In contrast to P and C individually, their composition CP can be defined given the Standard Model field content and could, in principle, be a symmetry.

2 Note that, while this equation is numerically correct, the left- and right-handed spinor indices are not treated correctly. However, this does not matter in purely four-component computations. For the correct treatment of spinor indices, cf. [171].

CP in the Standard Model

From the discussion of C and P in QED, a CP transformation should map a left-handed Weyl fermion to a right-handed Weyl fermion with the opposite charges of the original fields. This, however, can be achieved by mapping the field to its own complex conjugate. Thus, there is no obstruction due to the field content.[3] Hence, under CP a left-handed Weyl fermion is mapped to its own complex conjugate amended by a matrix taking care of the spinor indices,

$$\boldsymbol{CP}\,\boldsymbol{\lambda}_\alpha(x)\,\boldsymbol{CP}^{-1} = \mathrm{e}^{\mathrm{i}\,\gamma}\,\mathrm{i}(\sigma^0)_{\alpha\dot\beta}\,(\boldsymbol{\lambda}^\dagger)^{\dot\beta}(x_P) =: \mathrm{e}^{\mathrm{i}\,\gamma}\,(\boldsymbol{\lambda}^{CP})_\alpha(x_P)\,. \tag{1.13}$$

The CP transformation of the gauge bosons is given by

$$\boldsymbol{CP}\,\boldsymbol{A}^\mu_a(x)\,\boldsymbol{CP}^{-1} = \eta_a\,\varepsilon(\mu)\,\boldsymbol{A}^\mu_a(x_P) \qquad \text{(no sum over } a)\,, \tag{1.14}$$

where the signs η_a are defined such that [14]

$$\eta_a\,T^a = -(T^a)^* \qquad \text{(no sum over } a)\,, \tag{1.15}$$

and where T^a are the generators of the gauge symmetry. This transformation is henceforth called canonical CP transformation.

Although CP could thus, in principle, be a symmetry of Nature, this is not the case. It is explicitly broken by complex entries of the Yukawa couplings to the Higgs boson. Glossing over some details, this statement can be intuitively understood as follows: CP exchanges each field in the Standard Model Lagrangian with its complex conjugate, i.e. it maps an operator $\boldsymbol{O}$ in the Lagrangian to its Hermitian conjugate operator $\boldsymbol{O}^\dagger$, which is, of course, also present in the Lagrangian to ensure that the action is real. However, the coupling c of this operator can be any complex number such that

$$c\,\boldsymbol{O} \overset{CP}{\longmapsto} c\,\boldsymbol{O}^\dagger \tag{1.16}$$

under CP, while the conjugate of the original term is

$$c^*\,\boldsymbol{O}^\dagger\,. \tag{1.17}$$

The Lagrangian containing this term could only be CP invariant for real c. It is important to note, moreover, that such a transformation does not forbid couplings but restricts them to real values. These statements are made more precise in the following sections.

In the Standard Model Lagrangian, the relevant couplings are, as already stated, the Yukawa couplings of the fermions to the Higgs boson responsible for fermion masses after electroweak symmetry breaking. As some of the entries of the Yukawa matrices are unphysical, in the sense that they are unobservable, see the discussion in Chapter III, it is not easy to determine whether for a given set of couplings CP is broken or not. There are two ways how to proceed, which shall now be sketched for the quark sector.

Firstly, one can diagonalise the Yukawa matrices, determine the quark mass eigenstates and compute the CKM matrix. After removing as many phases as possible, in the pure SM only the Dirac CP phase δ_{CP} is left and CP is broken if and only if it is neither zero nor π. This procedure is somewhat tedious and, moreover, seems to introduce a basis dependence

3 As it turns out, this statement is only true when ignoring possible additional symmetries, as is explained below.

into the discussion of CP invariance. This basis dependence is, of course, only an artefact; the answer to the question whether CP is broken or unbroken does not depend on the way the Lagrangian is formulated.

This puzzle can easily be resolved. The quark fields come in three generations distinguished only by their mass. That is, there is a U(3) symmetry for each quark flavour that is explicitly broken by the Yukawa couplings. Instead of explicitly going to the mass eigenstate basis, one can use a so-called generalised CP transformation [172],

$$\boldsymbol{CP}\,(f_i)_\alpha(x)\,\boldsymbol{CP}^{-1} = U_f^{ij}\,(f_j^{CP})_\alpha(x_P)\,, \tag{1.18}$$

where $f = q, u^c, d^c$ and i, j label the generations. The matrices U_f can be assumed unitary without loss of generality. For now, the occurrence of these matrices can be understood as making up for not working in the mass eigenstate basis; this statement is made more precise below. If the mass eigenstate basis is connected to the chosen basis by matrices V_f, using

$$U_f := V_f V_f^T \tag{1.19}$$

in (1.18) is the same as going to the mass eigenstate basis, performing the CP transformation (1.13) there and transforming back to the original basis. This resolves the seeming basis dependence of CP invariance encountered in the first approach. Generalised CP transformations like (1.18) are discussed much more thoroughly below in Section VII.3.[4]

The Yukawa couplings can break some or all of the CP transformations of equation (1.18), and CP is truly broken only if all of them are broken. This observation leads to the second approach for the detection of CP violation. One examines so-called weak basis invariants [172–176], which are combinations of couplings of a model that are invariant under unitary rotations in flavour space. Viewing CP transformations as mappings of couplings of a given Lagrangian, some of the invariants change sign under CP. If any CP transformation is a symmetry, these invariants vanish, and, vice versa, if any of these invariants does not vanish for the couplings of a given model, all possible CP symmetries are broken.

Let us illustrate this for the SM. The CP odd weak basis invariant that can be built from the SM Yukawas is the so-called Jarlskog determinant [173]. It is defined by

$$J := \frac{1}{\mathrm{i}}\,\det\left([Y_u\,Y_u^\dagger,\,Y_d\,Y_d^\dagger]\right). \tag{1.20}$$

The Jarlskog determinant is real and invariant under basis transformations of the quark fields. Since the commutator of two matrices is traceless and since one can show[5] that for a traceless three-dimensional matrix $\det(A) = \frac{1}{3}\,\mathrm{tr}\,(A^3)$, one can write the Jarlskog determinant also as [172]

$$J = \frac{1}{3\,\mathrm{i}}\,\mathrm{tr}\left([Y_u\,Y_u^\dagger,\,Y_d\,Y_d^\dagger]^3\right). \tag{1.21}$$

4 In fact, the matrices U_f have to fulfil certain consistency conditions [14]. However, in this particular case of U(3) symmetries, all unitary matrices are admissible because each such matrix represents an inner automorphism of U(3). See Section VII.3 for a detailed explanation of these ideas.

5 The characteristic polynomial of a matrix A is $\chi_A(\lambda) = \det(\lambda\mathbb{1}_n - A) = (-1)^n \det A + O(\lambda)$. It can also be expressed by $\chi_A(\lambda) = \exp\left[\mathrm{tr}\,(\ln(\lambda\mathbb{1}_n - A))\right]$. Expanding this in λ and comparing coefficients, one can derive a formula for the determinant of matrices of dimension n as a polynomial of their trace. This formula simplifies significantly when the matrix is traceless.

The action of the generalised CP transformation (1.18) on the Lagrangian is equivalent to the replacement

$$Y_u \overset{CP}{\longmapsto} U_q\, Y_u^*\, U_{u^c}^\dagger\,, \tag{1.22}$$

$$Y_d \overset{CP}{\longmapsto} U_q\, Y_d^*\, U_{d^c}^\dagger \tag{1.23}$$

of the Yukawa couplings. The Jarlskog determinant hence transforms under CP as

$$J \overset{CP}{\longmapsto} \frac{1}{\mathrm{i}}\,\det\left([U_q\, Y_u^*\, Y_u^T\, U_q^\dagger,\, U_q\, Y_d^*\, Y_d^T\, U_q^\dagger]\right) = -J^* = -J\,. \tag{1.24}$$

This shows that if CP is conserved, the Jarlskog invariant vanishes and, thus, that $J \neq 0$ implies broken CP. In fact, in the pure SM, CP is conserved if and only if J vanishes [172].[6] Of course, the approach of CP odd weak basis invariants for the detection of CP violation in the SM is equivalent to the aforementioned one using invariance of the Lagrangian [173].

Turning back to the CP transformation of equation (1.18), one should note that it is more general than the canonical CP transformation of equation (1.13), which was obtained by direct analogy from the QED case. For arbitrary U_f, i.e. without assuming (1.19), there are additional CP transformations, and the question arises whether they are any different and whether they can consistently be imposed on a theory. This, in a certain sense, is the first occurrence of a true so-called generalised CP transformation. It turns out that, whereas in the Standard Model equation (1.18) with U_f from (1.19) is the only sensible generalisation of the QED CP transformation, the situation is far less clear in models of physics beyond the SM. This issue is discussed from both conceptional and mathematical viewpoints in the following after a brief interlude on the uniqueness of the definition of the inversion symmetries in general quantum field theories.

VII.2 Uniqueness of the definitions of P, T, C and CP

The only really fundamental inversion symmetry of quantum field theory is CPT.[7] As can be shown, any quantum field theory is invariant under this symmetry [178], which is represented by an anti-linear, unitary operator $\boldsymbol{\Theta}$ on Hilbert space. It acts as [179]

$$\begin{aligned}\boldsymbol{\Theta}\,\boldsymbol{\Phi}_{\alpha_1\cdots\alpha_n}{}^{\dot\beta_1\cdots\dot\beta_m}(x)\,\boldsymbol{\Theta}^{-1} &:= (-1)^m\,(-\mathrm{i})^F\,\left(\boldsymbol{\Phi}_{\alpha_1\cdots\alpha_n}{}^{\dot\beta_1\cdots\dot\beta_m}\right)^\dagger(-x)\\ &= (-1)^m\,(-\mathrm{i})^F\,(\boldsymbol{\Phi}^\dagger)_{\dot\alpha_1\cdots\dot\alpha_n}{}^{\beta_1\cdots\beta_m}(-x)\end{aligned} \tag{2.1}$$

on a general spinor field, where F is one for fermionic and zero for bosonic fields. Since $\boldsymbol{\Theta}$ is an anti-unitary operator it conjugates all couplings (including objects like γ and σ matrices) and, hence, effectively exchanges a term in the Lagrangian with its complex conjugate term. Therefore, any Lagrangian quantum field theory with a real Lagrangian is invariant under this transformation, independently of the additional symmetry content of the theory.[8]

It is also this CPT symmetry of quantum field theory that 'provides a precise correspondence between particles and anti-particles' [165] implying, for example, that they have

6 For an alternative proof that $J \neq 0$ is a necessary and sufficient condition for CP violation in the Standard Model, see [177].

7 At this point, it is advisable to view CPT just as a name for the transformation defined in (2.1) without trying to interpret it as a combination of charge conjugation, parity transformation and time reversal.

8 In fact, CPT invariance follows from much less restrictive assumptions, cf. e.g. [178, 179].

identical masses and decay rates. If this statement were to rely on a C or CP symmetry, it would not hold in the Standard Model, where both these symmetries are broken.

If one assumes invariance of a theory under a generalised CPT transformation, i.e. a CPT transformation amended by multiplication with a unitary matrix U acting on a set of fields like in (1.18) for CP, the resulting theory is invariant independently under the canonical CPT transformation (2.1) and under multiplication by U^*. Therefore, the concept of such a generalised CPT transformations is meaningless and CPT uniquely defined [14].

As the name suggests, it is in some cases possible to view CPT as the combination of three separate inversion symmetries: charge conjugation C, parity transformation P and time reversal T. This is true, for example, for QED, for which the transformations were described above in Section VII.1.1. However, this separation in three different transformations is not unique, cf. [180], and might not even make sense for a given theory. For example, none of the three transformations is independently a symmetry of the Standard Model. Even more importantly, C and P cannot even be implemented as transformations acting on the SM field content. Thus, in the SM one can at most split CPT into two parts, CP and T, which are, however, broken explicitly by the Yukawa couplings.

Thus, quite naturally the questions arise how to generalise the CP transformation to models of physics beyond the Standard Model, how unique a given splitting of CPT into CP and T is, and what restrictions one should impose on possible generalisations of this symmetry.[9] There are two different aspects of this question: the first concerns the mathematical consistency of such generalisations and of the definition of CP in general. This is reviewed in the following section. The second aspect concerns the physical interpretation, i.e. the question whether it makes sense to call a given mathematically consistent transformation CP or not. This question is taken up in Section VII.4.1.

VII.3 CP and automorphisms

Models of physics beyond the Standard Model usually have enlarged gauge or global symmetry groups, e.g. Grand Unified Theories or models with discrete flavour symmetries. Hence, it is important to understand the interplay of these symmetries with a possible generalised CP transformation. It is advantageous to split this task into separate discussions of continuous (gauge) symmetries and of discrete symmetries, although the final results are structurally very similar.

VII.3.1 Gauge symmetries

The conditions a CP transformation has to fulfil in order to be consistent with the gauge symmetry of a model were first derived by Grimus and Rebelo [14]. They were able to show the following. Let the CP transformation act on a multiplet of left-handed Weyl fermions λ_i residing in a representation with generators T^a of the gauge group L as[10]

$$\lambda_i(x) \xrightarrow{CP} U_{CP}^{ij} \lambda_j^{CP}(x_P)\,, \tag{3.1}$$

9 Generalisations of parity and charge conjugation individually are not discussed here because these symmetries are already broken by the matter content of the Standard Model. There are, however, so-called left-right symmetric models which make use of a generalised parity transformation [181–183].

10 For simplicity, the notation is changed from field operators to fields.

where U_{CP} is unitary. Let it, further, act on the gauge bosons as

$$A^\mu(x) \overset{CP}{\longmapsto} R_{ab}\, \varepsilon(\mu)\, A^\mu_b(x_P)\,, \tag{3.2}$$

where R is real and orthogonal. Demanding that the gauge coupling term be invariant, the CP transformation matrices U_{CP} and R must fulfil two conditions. Firstly, they are required to fulfil the consistency equation [14]

$$U_{CP}\, \left(-R_{ab}\, (T^b)^*\right)\, U^\dagger_{CP} = T_a\,. \tag{3.3}$$

Secondly, the map [14]

$$\begin{array}{rccc} \tau_R: & \mathfrak{l} & \to & \mathfrak{l}\,, \\ & T^a & \mapsto & R_{ab}\, T^b \end{array} \tag{3.4}$$

must be an automorphism of the Lie algebra $\mathfrak{l}$ of L.

This latter condition is very restrictive. It allows one to enumerate all possible CP transformations by looking at all automorphisms of the Lie algebra of the gauge group. However, not all automorphisms lead to transformations that can be considered CP transformations. In fact, Grimus and Rebelo [14] singled out the so-called contragredient automorphism as the only automorphism leading to a consistent physical CP transformation by demanding that all quantum numbers should be reversed. For more details on this condition, see the discussion in Section VII.13 and the original reference [14].

Note that CP transformations that differ by a symmetry transformation of the theory lead to physically identical results. Inner automorphisms of the Lie algebra, which lead to inner automorphisms of the Lie group and, therefore, to symmetry transformations, are thus irrelevant. That is, the relevant group (or, rather, Lie algebra) theoretical structure is the outer automorphism group, see Definition 12. All automorphisms in a given equivalence class of the outer automorphism group lead to physically identical CP transformations [14].

Under a change of basis

$$\lambda_i \mapsto \lambda'_i := V^{ij}\, \lambda_j \tag{3.5}$$

for the fermion fields, the CP transformation changes to [14]

$$U'_{CP} := V\, U_{CP}\, V^T\,. \tag{3.6}$$

Realising this is important for two reasons. Firstly, the equation shows that starting with a canonical CP transformation, i.e. $U_{CP} = \mathbb{1}$, in one basis, one usually ends up with a non-canonical transformation, i.e. $U_{CP} \neq \mathbb{1}$, in different bases. Hence, the seeming generalisation of CP by including a matrix U_{CP} is not facultative but necessary. This is also the formal explanation of the observations made in Section VII.1.2, i.e. of equation (1.18).

Secondly, since (3.6) is not a similarity transformation, it is not always possible to transform to a basis where U_{CP} is trivial [24], see also Section A.6.4. Thus, there can be CP transformations that yield physically different results from the canonical CP transformation. This situation arises also for the discrete group case discussed below.

As an example for the connection of CP to an automorphism, let the gauge group L be $\mathrm{SU}(N)$, with $N > 2$. The usual CP transformation, as used in the SM for $\mathrm{SU}(3)_\mathrm{C}$, corresponds to the Dynkin diagram automorphism of the Lie algebra A_{N-1} [14]. This maps the weight $(\Lambda^1, \Lambda^2, \dots, \Lambda^{N-1})$ to $(\Lambda^{N-1}, \Lambda^{N-2}, \dots, \Lambda^1)$ and is a representative of the unique outer automorphism class of A_{N-1}. As it turns out, it is more intuitive to choose as a representative of this class the contragredient automorphism sending $(\Lambda^1, \Lambda^2, \dots, \Lambda^{N-1})$ to $(-\Lambda^1, -\Lambda^2, \dots, -\Lambda^{N-1})$ [14], see also the discussion in Section VII.13.

VII.3.2 Discrete symmetries

The analysis was repeated for the case of discrete symmetries by Holthausen, Lindner and Schmidt [15] and Feruglio, Hagedorn and Ziegler [16]. Let G be the discrete symmetry under consideration. Holthausen, Lindner and Schmidt [15] assemble all scalar fields φ_i of a given model, which are assumed to transform in irreducible representations of G, together with their complex conjugates in a field vector Φ,

$$\Phi := (\varphi_1, \varphi_1^*, \dots, \varphi_n, \varphi_n^*)^T \tag{3.7}$$

such that a matrix W exists with [15, equation (2.5)]

$$\Phi^* = W\,\Phi \tag{3.8}$$

and $W^2 = \mathbb{1}$. To be precise, Holthausen, Lindner and Schmidt [15] make a distinction between fields in real representations, denoted φ_R, in pseudo-real representations, φ_P, and complex representations, φ_C, and define [15, equation (2.1)]

$$\Phi := (\varphi_R, \varphi_P, \varphi_P^*, \varphi_C, \varphi_C^*)^T\,. \tag{3.9}$$

This distinction is unnecessary, and, moreover, the definition (3.9) of Φ is actually inconsistent with the existence of a W fulfilling (3.8). It is true that for real scalar fields, which can only reside in real representations, one would not have to include the conjugate field in Φ as well for W to exist, but there can also be complex fields in real representations, which are not related to their complex conjugates by a linear transformation. Thus, the definition (3.7) consistent with (3.8) is used hereafter, assuming that this is what was actually desired by Holthausen, Lindner and Schmidt [15]. This assumption is strengthened by their claim that one should 'note that Φ always contains the field and its complex conjugate' [15].

The discrete group acts on Φ as

$$\Phi \overset{G}{\longmapsto} \rho_\Phi(g)\,\Phi\,, \qquad \forall\, g \in G\,, \tag{3.10}$$

where $\rho_\Phi(g)$ is a matrix realisation of the reducible representation $\boldsymbol{R}_\Phi$ of Φ under G. The generalised CP transformation is then written as[11]

$$\Phi \overset{CP}{\longmapsto} U_{CP}\,\Phi^* = U_{CP}\,W\,\Phi\,, \tag{3.11}$$

where the last part is only consistent for the definition of Φ adopted here.

The crucial constraint on the CP transformation is that performing first a CP transformation, then a discrete symmetry transformation and then an inverse CP transformation should not change the Lagrangian [15]. If this were not the case, i.e. if the Lagrangian were not mapped onto itself when performing these consecutive operations, the CP and discrete symmetry transformations would be mutually inconsistent. In fact, the transformation properties of the Lagrangian under G would depend on whether one first performs a CP transformation or not, which is clearly unphysical.

Since a Lagrangian is, by definition, only left invariant by a symmetry operation, the concatenation of the three operations must also be a symmetry operation; otherwise, the

11 From now on, only the transformation behaviour of scalar fields is shown and the change of the space-time dependence is suppressed. The transformation of fermion fields can be obtained if instead of the complex conjugate field the CP conjugate field defined analogously to equation (1.13) is used. This takes care of the Lorentz structure of the expression.

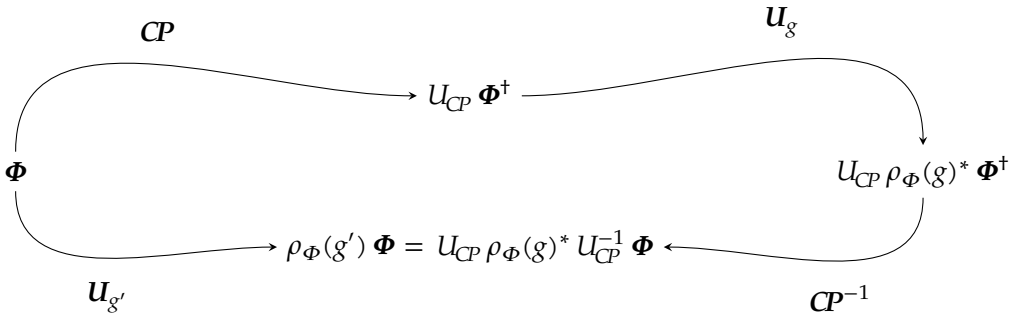


Figure VII.1: This is a reproduction of Figure 1 from [15], showing the consecutive operations of CP, $g \in G$ and inverse CP on a field operator Φ in comparison to just a symmetry transformation. Note that each of the consecutive operations acts on the field operator itself, cf. [184].

Lagrangian would not be left invariant. Assuming, furthermore, that G is the full symmetry group acting on the chosen representation space, one obtains the condition [15]

$$\forall\, g \in G : \exists\, g' \in G : U_{CP}\,\rho_\Phi(g)^*\,U_{CP}^{-1} = \rho_\Phi(g')\,. \tag{3.12}$$

This is also depicted in Figure VII.1. Further, R_Φ is a faithful representation because, otherwise, the symmetry group would not be G but rather the quotient group $G/\ker R_\Phi$. Thus, by taking the inverse image under ρ_Φ, equation (3.12) can be seen as a map from the group G into itself,[12]

$$\begin{aligned} u:\ G &\to G\,,\\ g &\mapsto g' := \rho_\Phi^{-1}\left(U_{CP}\,\rho_\Phi(g)^*\,U_{CP}^{-1}\right)\,. \end{aligned} \tag{3.13}$$

Moreover, it is clear that

$$\begin{aligned} u(g_1g_2) &= \rho_\Phi^{-1}\left(U_{CP}\,\rho_\Phi(g_1)^*\,\rho_\Phi(g_2)^*\,U_{CP}^{-1}\right)\\ &= \rho_\Phi^{-1}\left(U_{CP}\,\rho_\Phi(g_1)^*\,U_{CP}^{-1}\,U_{CP}\,\rho_\Phi(g_2)^*\,U_{CP}^{-1}\right)\\ &= \rho_\Phi^{-1}\left(U_{CP}\,\rho_\Phi(g_1)^*\,U_{CP}^{-1}\right)\,\rho_\Phi^{-1}\left(U_{CP}\,\rho_\Phi(g_2)^*\,U_{CP}^{-1}\right)\\ &= u(g_1)u(g_2)\,, \end{aligned} \tag{3.14}$$

i.e. u is a homomorphism of G. As there is also an inverse function for u,

$$\begin{aligned} u^{-1}:\ G &\to G\,,\\ g' &\mapsto g := \rho_\Phi^{-1}\left((U_{CP}^{-1})^*\,\rho_\Phi(g')^*\,U_{CP}^*\right)\,, \end{aligned} \tag{3.15}$$

the map u is, in fact, an automorphism of G [15]. Hence, one can rewrite equation (3.12) to the consistency equation [15]

$$\exists\, u \in \mathrm{Aut}(G) : U_{CP}\,\rho_\Phi(g)^*\,U_{CP}^{-1} = \rho_\Phi(u(g))\,, \qquad \forall\, g \in G\,, \tag{3.16}$$

for U_{CP}, which is the discrete group analogue to (3.3). Note that U_{CP} is only defined up to a phase by this relation. Finally, equation (3.6) is also the correct basis transformation for U_{CP} in the discrete group case.

12 Note that ρ_Φ^{-1} is the inverse of the map $\rho_\Phi : G \to \mathrm{GL}(n,\mathbb{C})$ and not the matrix inverse of a representation matrix, which would be denoted $\rho_\Phi(g)^{-1}$.

The structure of CP transformations in the presence of finite groups is thus reminiscent of the Lie group case discussed before. Again, the possible CP transformations are a subset of the automorphisms of the symmetry group G. In fact, CP transformations belonging to automorphisms that are connected by an inner automorphism, i.e.

$$u' \equiv \mathrm{conj}(c) \circ u \tag{3.17}$$

for some c in G, lead to CP transformations that are related by

$$U'_{CP} = \rho_\Phi(c)\, U_{CP}\,. \tag{3.18}$$

As $\rho_\Phi(c)$ is a symmetry transformation, the two CP transformations are indistinguishable. Hence, one can again restrict one's attention to the outer automorphism group $\mathrm{Out}(G)$ when enumerating possible CP transformations [15].

It is instructive to illustrate the failure of CP if equation (3.16) is not fulfilled by an example which was presented already in [15]. This example is based on the tetrahedral group A_4 with two scalar fields x and y each transforming in the triplet representation **3** and a scalar field φ transforming in the representation $\mathbf{1}_2$. The basis conventions are shown in Section A.1.1. Consider the term

$$c\left[\varphi \otimes (x \otimes y)_{\mathbf{1}_1}\right]_{\mathbf{1}_0} = c\,\varphi\,\frac{x_1\,y_1 + \omega^2\,x_2\,y_2 + \omega\,x_3\,y_3}{\sqrt{3}}\,, \tag{3.19}$$

which is a trivial A_4 singlet, i.e. an allowed term in an A_4 invariant Lagrangian with coupling c.[13] Under a canonical CP transformation, i.e. under just the replacement of each scalar field with its own complex conjugate, the resulting term is

$$c\left[\varphi \otimes (x \otimes y)_{\mathbf{1}_1}\right]_{\mathbf{1}_0} \xmapsto{CP} c\,\varphi^*\,\frac{x_1^*\,y_1^* + \omega^2\,x_2^*\,y_2^* + \omega\,x_3^*\,y_3^*}{\sqrt{3}}\,. \tag{3.20}$$

Comparing this to the complex conjugate of (3.19), one has to realise that there is no choice of coupling c for which the two terms coincide. That is, if insisting on both the A_4 symmetry and the canonical CP transformation, this term (and many others) is forbidden. In fact, the term (3.20) is not even A_4 invariant. This is a result of $U_{CP} = \mathbb{1}$ not being a solution to (3.16) for any automorphism of A_4. There is, however, the non-inner automorphism [15]

$$u: \quad (s,t) \quad \mapsto \quad (s,t^2)\,, \tag{3.21}$$

see Section A.1.1 for the A_4 notation, which yields

$$U_{CP} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{3.22}$$

for the triplets x and y. Thus, besides conjugating each scalar field, one should exchange the second and third components of the triplets x and y. This generalised CP transformation maps the term (3.19) to

$$c\left[\varphi \otimes (x \otimes y)_{\mathbf{1}_1}\right]_{\mathbf{1}_0} \xmapsto{CP} c\,\varphi^*\,\frac{x_1^*\,y_1^* + \omega^2\,x_3^*\,y_3^* + \omega\,x_2^*\,y_2^*}{\sqrt{3}}\,, \tag{3.23}$$

13 Note that, as usual, $\omega = \mathrm{e}^{2\pi\,\mathrm{i}\,/3}$.

which is precisely the same as the complex conjugate of (3.19) up to conjugation of the coupling c, which by the CP transformation is thus simply forced to be real.

Studying this example, it becomes clear that complex Clebsch–Gordan coefficients, e.g. here the ω, play a crucial role. This connection is explored in detail in Section VII.5. For A_4 the fact that a non-trivial U_{CP} is needed is not an intrinsic feature of the group but depends on the chosen basis. Indeed, one can find a basis in which U_{CP} is trivial for the given automorphism. However, as shown below, finding such a basis is not possible for all discrete groups.

In summary, it is known that any CP transformation of a given model has to fulfil one of the consistency conditions (3.3) and (3.16) depending on the type of group in question, which relates it to automorphisms of the group. However, in the discrete group case the question remains whether this argument can be reversed, i.e. whether each automorphism leads to a generalised CP transformation (for continuous groups, see [14] and Section VII.13). In fact, this turns out not to be the case. The reasons for this are discussed in the following section.

Before proceeding with the discussion, note that in addition to the action of CP on gauge and on discrete symmetry representations, one can also understand its action on the Lorentz indices from the discussion of automorphisms of the Lorentz group. As a matter of fact, parity, charge conjugation and time reversal were identified as automorphisms of the Lorentz group by Buchbinder, Gitman and Shelepin [168]. However, this is not dwelt on any further here.

VII.4 Proper CP for discrete groups

As detailed in the preceding section, Grimus and Rebelo [14] for Lie groups as well as Holthausen, Lindner and Schmidt [15] and Feruglio, Hagedorn and Ziegler [16] for discrete groups established that a CP transformation must be connected to an automorphism of the symmetry group. Further, they showed that only automorphisms which are not in the same equivalence class of the outer automorphism group give rise to physically distinct CP transformations. Thus, the possible CP transformations can be related to a subset of the outer automorphism group of the symmetry in question. However, this does not imply the converse: that any automorphism gives rise to a CP transformation. Whereas for continuous groups the relevant automorphisms were singled out by Grimus and Rebelo [14], no conditions were given for discrete groups. Indeed, it was claimed that 'there is a one-to-one correspondence between generalised CP transformations […] and the outer automorphism group' [15]. We would like to point out that this is not the case.

To this end, a closer inspection of the consistency condition (3.16) and of the definition (3.7) of Φ is necessary.[14] Given any representation $\boldsymbol{R}$ of G, the concatenation of $\boldsymbol{R}$ with an automorphism u of G is again a representation $\boldsymbol{R} \circ u$ of G because this is again a map from G to the general linear group of the representation space of $\boldsymbol{R}$. The dimensions of $\boldsymbol{R}$ and $\boldsymbol{R} \circ u$ are identical and from the character scalar product it is also clear that $\boldsymbol{R} \circ u$ is irreducible if and only if $\boldsymbol{R}$ is irreducible. Further, note that, given a specific matrix realisation ρ_R of $\boldsymbol{R}$,

14 Note that, as explained below equation (3.8), one might think that a different definition of Φ is used here than seemingly was employed by [15]. This, however, just remedies the fact that their definition did not fulfil their requirements on Φ. Moreover, the present definition is in accordance with their statement quoted below (3.9).

the map

$$\begin{array}{rccl} \rho_R^* : & G & \to & \mathrm{GL}(n,\mathbb{C})\,, \\ & g & \mapsto & \rho_R(g)^* \end{array} \tag{4.1}$$

yields a specific matrix realisation of the complex conjugate representation $\overline{\boldsymbol{R}}$, see Definition 18. This implies that the conjugate φ^* of a field φ in representation $\boldsymbol{R}$ transforms in the conjugate representation $\overline{\boldsymbol{R}}$ of $\boldsymbol{R}$.

Comparing to the Definition 20 of an intertwiner, the consistency condition (3.16) is nothing but the statement that the CP transformation has to be an intertwiner of $\overline{\boldsymbol{R}}_\Phi$ with $\boldsymbol{R}_\Phi \circ u$ for some automorphism u, i.e. equation (3.16) is equivalent to

$$\exists\, u \in \mathrm{Aut}(G) : \overline{\boldsymbol{R}}_\Phi \cong \boldsymbol{R}_\Phi \circ u\,. \tag{4.2}$$

If this condition is fulfilled, one can use equation (3.16) to compute the matrix U_{CP} in a specific basis. However, Schur's lemma (Theorem 9) places stringent constraints on the solvability of equation (4.2) because it states that for two irreducible representations there either is no intertwiner or the intertwiner is uniquely determined up to a phase.[15] We come back to this when categorising all solutions.

Returning to the reverse question whether each automorphism leads to a CP transformation, this can now be split into two sub-questions.

The first part is whether $\overline{\boldsymbol{R}}_\Phi \cong \boldsymbol{R}_\Phi \circ u$ is true for all automorphisms u. This is certainly not the case. As an example, let G be $\Delta(27)$ and $\Phi = (\varphi, \varphi^*)^T$ with φ transforming in representation $\mathbf{1}_1$, see Section A.1.3 for the notation. Then choose as automorphism

$$u_2 : \quad (a,b) \quad \mapsto \quad (aba, b) \quad . \tag{4.3}$$

As can be easily checked, this automorphism intertwines $\mathbf{1}_1$ with $\mathbf{1}_4$ and $\mathbf{1}_2$ with $\mathbf{1}_8$ whereas $\overline{\mathbf{1}}_1 \cong \mathbf{1}_2$. Since $\boldsymbol{R}_\Phi = \mathbf{1}_1 \oplus \mathbf{1}_2$, one finds that

$$\overline{\boldsymbol{R}}_\Phi = \overline{\mathbf{1}}_1 \oplus \overline{\mathbf{1}}_2 \cong \mathbf{1}_2 \oplus \mathbf{1}_1 \ncong \mathbf{1}_4 \oplus \mathbf{1}_8 \cong (\mathbf{1}_1 \oplus \mathbf{1}_2) \circ u = \boldsymbol{R}_\Phi \circ u\,. \tag{4.4}$$

Thus, as, in principle, already noted by Holthausen, Lindner and Schmidt [15], there is not always a solution to the consistency condition for a given model. This is in contradiction to their own statement cited above that there is a one-to-one correspondence between automorphisms and CP transformations.

Let us repeat this statement for emphasis. There is no one-to-one correspondence between CP transformations and automorphisms of a symmetry group because, as in the $\Delta(27)$ example presented, there are cases in which the field content is such that $\overline{\boldsymbol{R}}_\Phi \ncong \boldsymbol{R}_\Phi \circ u$.

Although this has, in principle, already settled the question, one can proceed one step and ask whether each automorphism u for which $\overline{\boldsymbol{R}}_\Phi \cong \boldsymbol{R}_\Phi \circ u$ gives rise to a proper CP transformation. This is a more subtle question which is sensitive to the precise definition of $\boldsymbol{R}_\Phi$. To understand why this is the case, let $\boldsymbol{R}$ be a complex irreducible representation of a discrete group G. Then the representation obtained by concatenating this with any inner automorphism is always equivalent to $\boldsymbol{R}$,

$$\boldsymbol{R} \circ \mathrm{conj}(c) \cong \boldsymbol{R}\,, \qquad \forall\, c \in G\,. \tag{4.5}$$

15 In principle, it is not a phase factor but multiplication with any non-zero complex number. However, the matrix representation of the intertwiner can always be chosen unitary and is then fixed up to a phase. This is always assumed implicitly in the following.

To prove this, one can compute the character, see Definition 21,

$$\chi_{R\circ\mathrm{conj}(c)}(g) = \chi_R(\mathrm{conj}(c)(g)) = \chi_R(g)\,, \qquad \forall\, g \in G\,, \tag{4.6}$$

where it has been used that characters are class functions. The desired result follows because characters are in one-to-one correspondence with representations. Now let φ be any field in a complex irreducible representation $\boldsymbol{r}$ of a group G such that $\Phi = (\varphi,\, \varphi^*)^T$ and

$$\boldsymbol{R}_\Phi = \boldsymbol{r} \oplus \bar{\boldsymbol{r}}\,. \tag{4.7}$$

This specific choice makes it possible that the consistency condition can be solved for any inner automorphism. Let, for example, u be the identity automorphism. Then

$$\overline{\boldsymbol{R}}_\Phi = \bar{\boldsymbol{r}} \oplus \boldsymbol{r} \cong \boldsymbol{r} \oplus \bar{\boldsymbol{r}} \cong (\boldsymbol{r} \oplus \bar{\boldsymbol{r}}) \circ \mathrm{id} = \boldsymbol{R}_\Phi \circ \mathrm{id}\,, \tag{4.8}$$

and analogously for any inner automorphism by the statement proved above. This solution is forced in the sense that it relies on the somewhat unusual inclusion of the conjugate field φ^* in the field vector Φ, and, in fact, one has to pay a price for this. The intertwiner in the (natural) basis where $\boldsymbol{R}_\Phi = \boldsymbol{r} \oplus \bar{\boldsymbol{r}}$ is block-diagonal for $u = \mathrm{id}$ is the matrix W from (3.8). Hence, the alleged CP transformation derived from (3.16) acting on Φ is

$$\Phi \longmapsto U_{CP}\, \Phi^* = W\, \Phi^* = \Phi\,. \tag{4.9}$$

This is, of course, no proper CP transformation. In fact, in the special case of the identity automorphism and the block-diagonal basis it is just the identity transformation and for any other inner automorphism it is just the corresponding discrete symmetry transformation. Thus, choosing Φ like Holthausen, Lindner and Schmidt [15] makes it possible to solve the consistency condition but it does by far not always lead to a CP transformation.

Even if one abandons the special case of inner automorphisms, something similar can happen. Consider again $\Delta(27)$ with a field φ which this time is to transform in the triplet representation **3**. The automorphism

$$u_5 : \quad (a, b) \quad \mapsto \quad (ba^2b^2, ab^2a^2) \tag{4.10}$$

is such that $\mathbf{3} \circ u_5 \cong \mathbf{3}$ and

$$\Phi \longmapsto U_{CP}\, \Phi = U\, W\, \Phi^* = U\, \Phi\,, \tag{4.11}$$

where U is, by Schur's lemma (Theorem 9), a block-diagonal matrix. In fact, $U = U_{u_5} \oplus U_{u_5}^*$ with

$$U_{u_5} = \begin{pmatrix} 0 & 0 & \omega^2 \\ 0 & 1 & 0 \\ \omega & 0 & 0 \end{pmatrix}. \tag{4.12}$$

Hence, the alleged CP transformation is non-trivial but does not amount to anything similar to CP as known from the SM (or any other theory). It is rather an additional discrete symmetry transformation enlarging $\Delta(27)$ to some larger symmetry group. Again, this is an artefact from the inclusion of the complex conjugate fields in Φ.

The consistency condition as proposed by Holthausen, Lindner and Schmidt [15] therefore does, if it can be solved, ensure consistency with the discrete symmetry group, but there is no intrinsic connection to CP.

Examining the various automorphisms of $\Delta(27)$ and their actions on irreducible representations, which are also shown in (A.1.21), one realises that there are several types of solutions, depending both on the field content of a model and on the chosen automorphism. Let us hence discuss the possible types of solutions to (3.16).

As mentioned earlier, the crucial constraint is Schur's lemma. By construction, the representation $\boldsymbol{R}_\Phi$ is a direct sum of the irreducible representations of all fields and their conjugate representations. According to Schur's lemma only equivalent irreducible representations can be intertwined (of course, this was precisely used to define the notion of equivalent representations) and the dimension of the space of their intertwiners is one. If there are no two fields in identical or mutually complex conjugate representations, i.e. if the decomposition of $\boldsymbol{R}_\Phi$ into irreducible representations is free of duplicates, and provided there is a solution at all, the full intertwiner of $\overline{\boldsymbol{R}}_\Phi$ and $\boldsymbol{R}_\Phi \circ u$ spelt out in its matrix form U_{CP} consists of blocks for each of the irreducible components of $\boldsymbol{R}_\Phi$. The transformation (3.11) can thus be written as

$$\varphi_i \longmapsto U_{CP}(\varphi_i)\, \varphi_j^{(*)}\,, \qquad \forall\, i\,, \tag{4.13}$$

i.e. each field in an irreducible representation is mapped to the same ($i = j$) or a different ($i \neq j$) field, conjugated or not, and multiplied with a possibly trivial matrix $U_{CP}(\varphi_i)$, which is uniquely determined up to a phase. If there are several fields in the same irreducible representation, i.e. if the decomposition of $\boldsymbol{R}_\Phi$ is not multiplicity free, they can, in addition, be rotated into each other by a unitary transformation which is left undetermined by (3.16). This is equivalent to the statement in Schur's lemma that the space of intertwiners has as dimension the number of equivalent irreducible constituents, see Theorem 9.

Building on these general considerations, let us list the different types of solutions to the consistency equation (3.16); the reasoning behind the (telling) names is explained in detail below.

Proper (generalised) CP: Every field is sent to its own complex conjugate and multiplied by a (possibly trivial) matrix,

$$\varphi_i \longmapsto U_{CP}(\varphi_i)\, \varphi_i^*\,, \qquad \forall\, i\,. \tag{4.14}$$

Here and in the following, $U_{CP}(\varphi_i)$ denotes the matrix obtained from equation (3.16) for the field φ_i.

Extended proper CP: Every field is sent to the complex conjugate of a possibly different field in the same representation and multiplied by a (possibly trivial) matrix,

$$\varphi_i \longmapsto U_{CP}(\varphi_i)\, \varphi_j^*\,, \qquad \forall\, i\,. \tag{4.15}$$

This type is structurally identical to the first type because the representations of φ_i and φ_j are the same (otherwise, this transformation would not solve the consistency condition, see the discussion above).

Discrete symmetry: Every field is sent to itself and multiplied by a (possibly trivial) matrix,

$$\varphi_i \longmapsto U_{CP}(\varphi_i)\, \varphi_i\,, \qquad \forall\, i\,. \tag{4.16}$$

Hence, the transformation just acts as an ordinary discrete symmetry.

CP-like: Some fields are sent to complex conjugated fields and some fields are sent to non-conjugated fields. That is, this type is a mixture of an (extended) proper CP and a discrete symmetry. Note that, if no field is sent to its own complex conjugate, one can arrive at a discrete symmetry type transformation by adjusting the conventions on which field is called conjugate, i.e. by exchanging the notation $\varphi^* \leftrightarrow \varphi$. Hence, in the following it is assumed that this freedom is used to reduce the transformation to the discrete symmetry type whenever possible, and a transformation is only called CP-like if this reduction is impossible.

After identifying these different types of transformations as possible solutions to the consistency condition (3.16), one can determine which of them should be considered proper physical CP transformations.

VII.4.1 Physically motivated conditions on CP

The goal of any model of physics beyond the Standard Model is to provide an explanation for some of the unsolved problems of the SM, e.g. solve the flavour puzzle. Of course, this implies that the low-energy limit of such a theory should be the SM. Applied to CP, the low-energy remnant of any generalised CP transformation should lead to a consistent CP transformation for the effective SM as shown in (1.18). Let us now discuss this for the different types of transformation behaviours described above.

Discrete symmetry

The transformations termed 'discrete symmetry' above, where no field is conjugated, do certainly not fulfil the criterion that they can lead to a proper SM CP transformation in the low-energy limit. Rather, these transformations are, as also seen in the example discussed before, just what the name suggests: additional discrete symmetry transformations. For example, one could start with an A_4 model, impose such a solution to the consistency equation as a symmetry, and end up with an S_4 model. This enlarged symmetry can change model predictions, but there is no connection whatsoever to CP. Thus, any such solution should be discarded when looking for generalisations of CP.

Proper generalised CP

The opposite situation is what was called 'proper generalised CP'. In this case, each irreducible multiplet is sent to its own conjugate and multiplied by some matrix which can be obtained from (3.16). This clearly mimics the CP transformation (1.18). In fact, putting the quarks, say, in some three-dimensional representation of a discrete group G, the consistency equation just puts a constraint on what kind of matrices are allowed in (1.18), depending on the structure of G and the chosen automorphism. Any such transformation would thus lead to a zero Jarlskog determinant, i.e. CP invariance, in perfect accordance with the discussion of CP in the SM. Moreover, the action of such a transformation on the Baryon number operator is, of course, also as known from the SM, cf. e.g. [185], i.e. without violating this symmetry no Baryon asymmetry could arise [34]. It is hence clear that, on the present level of the discussion, this class of transformations deserves its name and should be considered a valid generalisation of CP to models with discrete symmetries. Note that one can also try to define CP as inversion of quantum numbers as done for continuous groups by Grimus

and Rebelo [14]. This is discussed in Section VII.13. However, it turns out that this does not lead to any new unambiguous constraints on CP transformations besides the present ones.

The 'extended proper CP' transformations are from the group theory viewpoint no different from the non-extended 'proper CP' transformations. However, exchanging, for example, two particles transforming in the same representation of G can, of course, have effects on the phenomenology of a model. Since such statements obviously depend on the model rather than on the group theory and since any 'extended proper CP' transformation can be replaced by a non-extended one, this type of transformation is not discussed explicitly any further.

CP-like transformations

'CP-like' transformations are the most subtle type. Let us first repeat, however, that using the freedom to rename a conjugate field φ^* to φ, one can change the appearance of a transformation. For example, let the transformation be such that

$$\varphi_i \longmapsto \varphi_j^* \,, \qquad i \neq j \,, \tag{4.17}$$

which looks like part of an 'extended proper CP' transformation. Renaming $\varphi_j \leftrightarrow \varphi_j^*$ this reads

$$\varphi_i \longmapsto \varphi_j \,, \tag{4.18}$$

i.e. it looks like a discrete symmetry transformation. If no field in an irreducible representation is mapped to its own complex conjugate (perhaps multiplied by a matrix), one can use this freedom to reduce the transformation to a discrete symmetry transformation. In this case, this is not a CP transformation even though it might have looked like one before the relabelling.[16]

Thus, the only real 'CP-like' transformations are such that one or several fields are mapped to their own complex conjugates without all mappings obeying the more stringent constraints of an '(extended) proper CP' transformation. These cases are rather difficult to judge.

If any SM field, which might be a subset of some larger discrete symmetry representation, is not sent to its own complex conjugate, the transformation does certainly not resemble CP. In particular, if this is the case for a quark field, the Jarlskog determinant is not forced to vanish and Baryogenesis could occur without breaking this transformation.

However, one can also imagine the case that all fields giving rise to Standard Model fields after breaking of the additional discrete symmetry are mapped to their own complex conjugates by the transformation under consideration. Only some additional fields, e.g. flavons, would have an unusual transformation behaviour. It seems impossible to completely rule out this case just by analogy to the SM.

Nonetheless, there are some valid objections even to this case. The first is that the two sectors of fields with a proper and an improper transformation behaviour, respectively, are

16 In the simple case of an order two CP transformation, this is obvious. If the CP transformation only closes after several applications, i.e. $CP^n = \mathrm{id}$ only for n greater than two, this is somewhat less trivial. However, in any orbit obtained by applying CP consecutively to a given field until one arrives again at the original field, the number of different fields appearing involved is the same as the number of mappings, and any field shows up in precisely one such orbit. That is, the number of possible re-labellings is as large as the number of conditions from the mappings, and one can always rewrite the map into a discrete symmetry transformation.

to a certain degree decoupled. To illustrate this, assume there are two operators $O_{1/2}$ made up of one or several fields such that some contraction

$$O_1\, O_2 \tag{4.19}$$

is an invariant of the discrete group. If the CP-like transformation is such that

$$O_1 \longmapsto O_1\,, \tag{4.20a}$$
$$O_2 \longmapsto O_2^\dagger\,, \tag{4.20b}$$

the product of the two operators is neither mapped to its Hermitian conjugate nor to itself but

$$O_1\, O_2 \longmapsto O_1\, O_2^\dagger\,. \tag{4.21}$$

If O_2 does not transform in a real representation under all symmetries, $O_1\, O_2^\dagger$ is forbidden by a symmetry if $O_1\, O_2$ is allowed. Thus, $O_1\, O_2$ is forbidden by the CP-like transformation.

Let us illustrate this with an example. Take $O_1 = \varphi_1$ and $O_2 = \varphi_2$, where $\varphi_{1/2}$ are multiplets of the discrete group G. If the two fields are oppositely charged under a global $\mathrm{U}(1)$ symmetry such that their product is invariant, the CP-like transformed term is forbidden by the $\mathrm{U}(1)$ symmetry.[17] The term $\varphi_1\, \varphi_2$ thus would have to be absent from the Lagrangian.

Moreover, the two fields could not share any gauge quantum number because, if they were coupling to the same gauge bosons, only one of the two couplings could be invariant under the CP-like transformation; for the other term the transformation behaviour of the gauge bosons would be wrong. To be precise, let the $\mathrm{U}(1)$ symmetry from before be gauged. Then the gauge boson would have to transform trivially for the φ_1 gauge coupling to be non-zero and to transform like (1.14) for the φ_2 gauge coupling to be allowed.

In addition to that, the arguments on CP as inversion of quantum numbers presented in Section VII.13 below also single out the case of 'proper generalised CP' transformations as the only valid type.

For all these reasons, it seems justified only to call transformations fulfilling the criteria of 'proper generalised CP' transformations CP transformations at all and dismiss all the other types from the discussion. This result has profound consequences that are presented in the following.

VII.4.2 The refined consistency condition

The physical arguments of the preceding section single out the transformation behaviour of what was called 'proper generalised CP' transformations as the only valid generalisation of CP to models with discrete symmetries. One can feed this back into the consistency equation to obtain constraints on the automorphisms that can be used to define a CP transformation.[18] A CP transformation of the required form

$$\varphi_i \overset{CP}{\longmapsto} U_{CP}(\varphi_i)\, \varphi_i^*\,, \qquad \forall\, i\,, \tag{4.22}$$

17 This can also be understood using the result of Grimus and Rebelo [14] because the transformation of φ_1 does not obey their criteria for a CP transformation of the $\mathrm{U}(1)$ symmetry.

18 The specifications 'proper' and 'generalised' are dropped hereafter since only transformations fulfilling the corresponding criteria are considered CP transformations.

means that the matrix U_{CP} in (3.16) is block-diagonal. Thus, the single blocks $U_{CP}(\varphi_i)$ are solutions to a new, refined consistency condition,

$$\exists\, u \in \mathrm{Aut}(G) : U_{CP}(\varphi_i)\, \rho_{\boldsymbol{R}_{\varphi_i}}(g)^*\, U_{CP}(\varphi_i)^{-1} = \rho_{\boldsymbol{R}_{\varphi_i}}(u(g))\,, \qquad \forall\, g \in G\,,\, \forall\, i\,, \tag{4.23}$$

where $\boldsymbol{R}_{\varphi_i}$ is the irreducible representation of φ_i. Let us, furthermore, assume that the representation content of a model, i.e. the set of inequivalent irreducible representations that at least one field of the model resides in, is the full set of irreducible representations of the group G. In fact, depending on the group this assumption is stronger than needed, as can be seen in an example below. Furthermore, one can replace this assumption by the requirement that the CP transformation should be independent of the actual field content of a model. Then equation (4.23) can be read as an equation for each irreducible representation $\boldsymbol{R}_i$ of the group G:

$$\exists\, u \in \mathrm{Aut}(G) : U_i\, \rho_{\boldsymbol{R}_i}(g)^*\, U_i^{-1} = \rho_{\boldsymbol{R}_i}(u(g))\,, \qquad \forall\, g \in G\,,\, \forall\, i\,. \tag{4.24}$$

Note that the U_i are always chosen unitary here. The matrix U_{CP} as defined by Holthausen, Lindner and Schmidt [15], i.e. the transformation matrix of Φ, is then a block-diagonal matrix, where each block up to a phase only depends on the type of representation that the corresponding field transforms in.

The refined consistency condition (4.24) poses stringent constraints on the available automorphisms u.

u is class-inverting

Taking the trace of equation (4.24), one obtains the relation

$$\chi_{\boldsymbol{R}_i}(g^{-1}) = \chi_{\boldsymbol{R}_i}(g)^* = \mathrm{tr}\left(\rho_{\boldsymbol{R}_i}(g)\right)^* = \mathrm{tr}\left(\rho_{\boldsymbol{R}_i}(u(g))\right) = \chi_{\boldsymbol{R}_i}(u(g))\,, \qquad \forall\, g \in G\,,\, \forall\, i\,, \tag{4.25}$$

for the characters of the irreducible representations $\boldsymbol{R}_i$ of G.

An automorphism τ of G is said to be class-inverting if and only if $\tau(g)$ is in the same conjugacy class as g^{-1} for all g in G, cf. [186, 187]. Since group characters separate the conjugacy classes, see the remark below Definition 22, any u fulfilling (4.24) has to be class-inverting. This can also be turned around. Any class-inverting automorphism, i.e. any automorphism fulfilling (4.25), allows for a solution to equation (4.24). This is a simple consequence of the bijective correspondence between irreducible characters and irreducible representations, see Definition 21. The matrices U_i are just the corresponding intertwiners in the chosen basis. A GAP code determining whether an automorphism is class-inverting is shown in Appendix C.

Let us introduce some more terminology following [186]. A conjugacy class is called real if and only if its elements are conjugate to their inverse elements. If a group has only real conjugacy classes, it is called ambivalent, and any inner automorphism is class-inverting. This is equivalent to all irreducible characters of the group being real. A class-inverting automorphism either acts class-preservingly on a conjugacy class, which is then necessarily a real class, or it interchanges this conjugacy class with its inverse conjugacy class. Hence, a class-inverting automorphism can have odd order only for ambivalent groups.

Restrictions on the order of u

Applying a CP transformation twice to fields $\varphi_{\boldsymbol{R}_i}$ transforming in the irreducible representations $\boldsymbol{R}_i$ yields

$$\varphi_{\boldsymbol{R}_i} \overset{CP}{\longmapsto} U_i\,\varphi^*_{\boldsymbol{R}_i} \overset{CP}{\longmapsto} U_i\,U_i^*\,\varphi_{\boldsymbol{R}_i} =: V_i\,\varphi_{\boldsymbol{R}_i}\,,\ \forall\, i\,, \tag{4.26}$$

where V_i fulfils

$$V_i\,\rho_{\boldsymbol{R}_i}(g)\,V_i^{-1} = U_i\,\rho_{\boldsymbol{R}_i}(u(g))^*\,U_i^{-1} = \rho_{\boldsymbol{R}_i}(u^2(g)) = \rho_{\boldsymbol{R}_i}(v(g))\,, \qquad \forall\, g\in G\,,\ \forall\, i\,, \tag{4.27}$$

with $v := u^2$, which is a class-preserving automorphism. If the CP transformation is a symmetry, the square of it is also a symmetry. Thus, by introducing a CP symmetry, one might effectively end up with a larger discrete symmetry group than desired.

For the following discussion, it is convenient to distinguish three different cases.

(i) v is the identity automorphism,

(ii) v is an inner automorphism but not the identity, and

(iii) v is not an inner automorphism.

If v is the identity automorphism, $u^2 = \mathrm{id}$ and u is said to be involutory. One can show that this assumption is equivalent to $V_i = \pm\mathbb{1}$ for all i.

Plugging the assumption $v = \mathrm{id}$ into equation (4.27) shows that each V_i is a self-intertwiner for the irreducible representation $\boldsymbol{R}_i$. Thus,

$$V_i = \mathrm{e}^{\mathrm{i}\,\alpha_i}\,\mathbb{1} \Leftrightarrow U_i = \mathrm{e}^{\mathrm{i}\,\alpha_i}\,U_i^T\,, \qquad \forall\, i\,. \tag{4.28}$$

This is only possible if the phases α_i are either zero or π, i.e. $V_i = \pm\mathbb{1}$ and the U_i are either symmetric $(+)$ or anti-symmetric $(-)$. The reverse direction follows directly from (4.27) by plugging in $V_i = \pm\mathbb{1}$ and using the fact that all irreducible representations taken together, i.e. their direct sum, are faithful.[19]

One can thus conclude that if an involutory, class-inverting automorphism u is chosen in order to obtain a CP transformation, the discrete group G is either not enlarged at all or only enlarged to the direct product $G\times\mathbb{Z}_2$, where the charges of fields under the $\mathbb{Z}_2$ are determined by their irreducible G representation as $\mathrm{sign}(V_i)$. This case is illustrated with an example in Section VII.9.2. Note that groups with class-inverting, involutory automorphisms that are not ambivalent are called quasi-ambivalent, cf. [187].

The second case to be considered is that u squares to a non-trivial inner automorphism v, which implies that $\mathrm{ord}\,u > 2$. It turns out that such automorphisms seem not to make any predictions that are physically distinct from automorphisms of order two. The reason is that, as verified by an explicit computation with GAP, no group up to order 300 (with some exceptions that could not be checked, see Section A.4.1) has a class-inverting automorphism that is not connected to an involutory, class-inverting automorphism via an inner automorphism. For automorphisms of order $\mathrm{ord}\,(u) = 4m+2$ for integer m, of odd order, and for all automorphisms of odd-order groups, it is even proved in Section A.4.1 that such a correspondence exists. Here, being connected to a class-inverting, involutory

19 The implication that $V = \mathbb{1}$ means $u^2 = \mathrm{id}$ has also been realised in [188]. However, the other direction was not considered; in particular, it was not realised that an involutory automorphism can lead to V_i different from the unit matrix.

automorphism means that the composition of the given automorphism with some inner automorphism as described in equation (3.17) is class-inverting and involutory. As the corresponding CP transformations differ only by a symmetry transformation, see equation (3.18), their physical predictions are identical. Thus, it does not make much sense to discuss the class of higher-order class-inverting automorphism that square to an inner automorphism separately.

The last case is that the automorphism u does not square to an inner automorphism. Note that there really are class-preserving automorphisms that are not inner automorphisms, see e.g. group SG(32,43).[20] Again, no example for such a class-inverting automorphism that is not linked to an involutory, class-inverting automorphism has been found in the scan up to order 300. If such a case exists at all, the resulting discrete symmetry group $H = G \rtimes_v \mathbb{Z}_{\mathrm{ord}(v)}$ is a non-trivial semi-direct product as proved in Section A.4.2. However, the irreducible representations of G are contained in irreducible representations of H of the same dimension, i.e. one does not have to add further fields to obtain a viable model, and the additional symmetry only forbids couplings. Nonetheless, the behaviour of this case is not desired because the discrete symmetry group is non-trivially enlarged by introducing the CP symmetry. For this reason, and because no case is known at all, this type of automorphism is not considered any further.

Thus, to conclude, only class-inverting automorphisms can be used to obtain proper CP transformations. Moreover, for all practical purposes, one can restrict one's attention to involutory automorphisms.

After establishing these constraints on possible CP transformations, the connection of CP violation to complex Clebsch–Gordan coefficients is explained in the following section.

VII.5 Bickerstaff–Damhus automorphisms

Bickerstaff and Damhus [164] showed that a given set of matrix realisations $\rho_{\boldsymbol{R}_i}(g)$ of the irreducible representations $\boldsymbol{R}_i$ of a non-abelian finite group G allows for completely real Clebsch–Gordan coefficients[21] if and only if there exists an automorphism τ of G that satisfies

$$\rho_{\boldsymbol{R}_i}(g)^* = \rho_{\boldsymbol{R}_i}(\tau(g))\,, \qquad \forall\, g \in G\,,\ \forall\, i\,. \tag{5.1}$$

This looks like a special version of the consistency condition (4.24). By inserting equation (5.1) into itself it follows that the automorphism τ is involutory and taking the trace one sees that τ is class-inverting.

If there is an automorphism fulfilling (5.1) for a given basis, it is unique [164]. This can be proved in the following way. Let τ and τ' be two automorphisms of G which both fulfil equation (5.1) for the same matrix realisations $\rho_{\boldsymbol{R}_i}(g)$ of the irreducible representations $\boldsymbol{R}_i$. Then

$$\rho_{\boldsymbol{R}_i}(\tau(g)) = \rho_{\boldsymbol{R}_i}(g)^* = \rho_{\boldsymbol{R}_i}(\tau'(g))\,, \qquad \forall\, g \in G\,,\ \forall\, i\,. \tag{5.2}$$

Since the combination of all irreducible representations is faithful, their combined pre-image is unique and

$$\tau(g) = \tau'(g)\,, \qquad \forall\, g \in G\,. \tag{5.3}$$

20 The notation SG(*i*,*j*) denotes the *j*-th group of order *i* in the SmallGroups library of GAP, i.e. the numbers in parenthesis are the group's SmallGroups ID.

21 One can, of course, introduce superfluous phases by the phase rotations discussed in Section II.6.

However, the statement of (5.1) depends explicitly on the chosen basis. Transforming to a different basis $\rho'_{\boldsymbol{R}_i}(g) = S_i\,\rho_{\boldsymbol{R}_i}(g)\,S_i^\dagger$, equation (5.1) reads

$$\rho'_{\boldsymbol{R}_i}(\tau(g)) = (S_i\,S_i^T)\,\rho'_{\boldsymbol{R}_i}(g)^*\,(S_i\,S_i^T)^\dagger =: U_i\,\rho'_{\boldsymbol{R}_i}(g)^*\,U_i^\dagger\,, \qquad \forall\, g \in G\,,\ \forall\, i\,. \tag{5.4}$$

This is precisely the consistency condition (4.24) with the additional requirement that all matrices U_i should be symmetric. That is, if and only if the condition

$$\exists\,\tau \in \mathrm{Aut}(G) : \rho'_{\boldsymbol{R}_i}(\tau(g)) = U_i\,\rho'_{\boldsymbol{R}_i}(g)^*\,U_i^\dagger\,, \qquad U_i \text{ symmetric}, \qquad \forall\, g \in G\,,\ \forall\, i\,. \tag{5.5}$$

is fulfilled, there is a basis of G in which one can choose all Clebsch–Gordan coefficients to be real. In fact, this is then true in all bases for which all $U_i = \mathbb{1}$ for the given automorphism τ. These bases are connected by orthogonal basis transformations S_i.

Note that, while an automorphism fulfilling (5.1) for a given basis is uniquely determined, the basis-dependence implies that there can be several automorphisms fulfilling the condition (5.1) for different bases.[22] Using alternatively the condition (5.5) and fixing a basis, there can be several different sets of U_i which solve the equation for different automorphisms.

Any automorphism τ fulfilling (5.5) is henceforth called Bickerstaff–Damhus automorphism. As equation (5.5) is more stringent than the consistency condition (4.24), any Bickerstaff–Damhus automorphism defines a proper CP transformation. In fact, in the basis where equation (5.1) holds, this CP transformation is the canonical CP transformation with $U_{CP} = \mathbb{1}$. However, the reverse direction is not always true as was seen earlier; not every class-inverting, involutory automorphism is a Bickerstaff–Damhus automorphism because the corresponding U_i can be anti-symmetric.

The result by Bickerstaff and Damhus [164] implies that non-quasi-ambivalent groups do not admit any basis with completely real Clebsch–Gordan coefficients. In particular, non-abelian groups of odd order do not have such a basis. The proof of this statement can be found in Section A.4.3.

Although quasi-ambivalence is, in general, only a necessary condition for a basis with real Clebsch–Gordan coefficients, there are some groups for which it is also sufficient. This is the case for groups with only odd-dimensional irreducible representations [189]. The reason is that there is no anti-symmetric unitary, i.e. invertible, matrix in odd dimensions. Hence, given any involutory, class-inverting automorphism for such a group, all corresponding matrices U_i are symmetric, i.e. the automorphism is a Bickerstaff–Damhus automorphism. In summary, any quasi-ambivalent group with only odd-dimensional irreducible representations allows a choice of basis where the Clebsch–Gordan coefficients are real. An example where this can be applied is the tetrahedral group A_4.

Another special case are ambivalent groups. They have at least one Bickerstaff–Damhus automorphism if there is a group element $g \in G$ such that its characters are [189]

$$\chi_{\boldsymbol{R}_i}(g) = \begin{cases} \dim \boldsymbol{R}_i\,, & \boldsymbol{R}_i \text{ real} \\ -\dim \boldsymbol{R}_i\,, & \boldsymbol{R}_i \text{ pseudo-real} \end{cases}, \qquad \forall\, i\,. \tag{5.6}$$

In all other cases, one has to verify explicitly whether there is a Bickerstaff–Damhus automorphism and thus a basis with real Clebsch–Gordan coefficients. In the next section, a tool is introduced to greatly simplify this task.

22 For example, the group SG(64,109) has two distinct Bickerstaff–Damhus automorphisms that are both not inner and that also do not differ by an inner automorphism. For other examples, see the list in Appendix D.

VII.6 Twisted Frobenius–Schur indicator

One disadvantage of equation (5.5) is that it explicitly requires the representation matrices for all irreducible representations of a group. There is, however, also a possibility to check whether a given automorphism is a Bickerstaff–Damhus automorphism that only requires the characters of the group. The desired tool is the so-called twisted Frobenius–Schur indicator [164, 190].

In analogy to the (ordinary) Frobenius–Schur indicator presented in Theorem 12, the twisted Frobenius–Schur indicator for an irreducible representation $\boldsymbol{R}_i$ of a finite group G and an automorphism τ of this group is defined by

$$\mathrm{FS}_\tau(\boldsymbol{R}) := \frac{1}{|G|} \sum_{g\in G} \chi_{\boldsymbol{R}}(g\tau(g)) \,. \tag{6.1}$$

A GAP code implementing this definition can be found in Appendix C. Applied to all irreducible representations $\boldsymbol{R}_i$, it assumes the values

$$\mathrm{FS}_\tau(\boldsymbol{R}_i) = \begin{cases} 1\,,\ \forall\, i\,, & \text{if } \tau \text{ is a Bickerstaff–Damhus automorphism,} \\ \pm 1\,,\ \forall\, i\,, & \text{if } \tau \text{ is class-inverting and involutory,} \end{cases} \tag{6.2a}$$

but

$$\exists\, i : \mathrm{FS}_\tau(\boldsymbol{R}_i) \neq \pm 1 \qquad \text{if } \tau \text{ is not class-inverting and/or not involutory.} \tag{6.2b}$$

Together with the results of the previous section, the twisted Frobenius–Schur indicator can be used to determine whether a given automorphism is a Bickerstaff–Damhus automorphism. By checking all automorphisms of a group G, one can thus determine whether this group allows for a basis with real Clebsch–Gordan coefficients. A sequence of steps to determine whether a group has such a basis is shown in Figure VII.2.

In order to prove the statement (6.2), write the definition of the twisted Frobenius–Schur indicator in terms of matrix components of an arbitrary (unitary) basis of $\boldsymbol{R}_i$,

$$\mathrm{FS}_\tau(\boldsymbol{R}_i) = \frac{1}{|G|} \sum_{g\in G} \left[\rho_{\boldsymbol{R}_i}(g)\right]_{km} \left[\rho_{\boldsymbol{R}_i}(\tau(g))\right]_{mk} . \tag{6.3}$$

In this form, one can apply the Schur orthogonality relations of Theorem 10. As explained in Section VII.4.2, the irreducible representations realised by $\rho_{\boldsymbol{R}_i}(g)$ and $\rho_{\boldsymbol{R}_i}(\tau(g))^*$ are equivalent for all i if and only if τ is class-inverting. Hence, if τ is not class-inverting, according to Theorem 10, the twisted Frobenius–Schur indicator vanishes for at least one irreducible representation, proving the last point of (6.2).

Let now τ be class-inverting. Then the consistency equation (4.24) has a solution, i.e. there is a unitary matrix U_i for each irreducible representation $\boldsymbol{R}_i$ such that

$$U_i\, \rho_{\boldsymbol{R}_i}(g)^*\, U_i^{-1} = \rho_{\boldsymbol{R}_i}(\tau(g))\,, \qquad \forall\, g \in G\,,\ \forall\, i\,. \tag{6.4}$$

Inserting this into the twisted Frobenius–Schur indicator and simplifying the expression one arrives at

$$\begin{aligned} \mathrm{FS}_\tau(\boldsymbol{R}_i) &= \frac{1}{|G|} \sum_{g\in G} \left[\rho_{\boldsymbol{R}_i}(g)\right]_{km} [U_i]_{ma} \left[\rho_{\boldsymbol{R}_i}(g)^*\right]_{ab} [U_i^{-1}]_{bk} \\ &= \frac{1}{\dim \boldsymbol{R}_i}\, \delta_{ka}\, \delta_{mb}\, [U_i]_{ma}\, [U_i^*]_{kb} \\ &= \frac{1}{\dim \boldsymbol{R}_i}\, \mathrm{tr}\left(U_i^*\, U_i\right). \end{aligned} \tag{6.5}$$

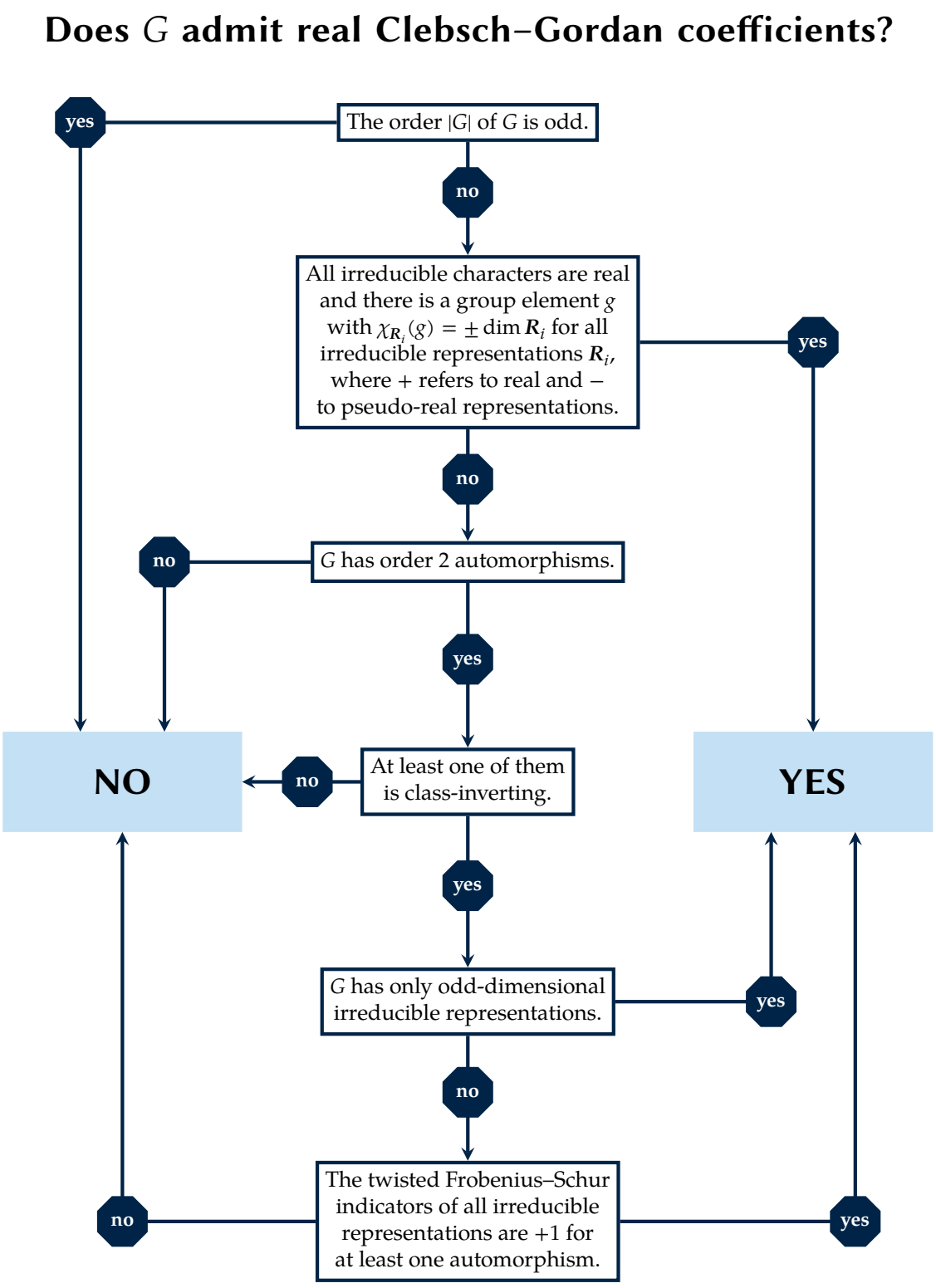


Figure VII.2: This is a schematic overview of the steps one could follow to determine whether a finite non-abelian group G admits real Clebsch–Gordan coefficients.

As already shown in Section VII.4.2, if τ is an involution, then each of the U_i is either symmetric or anti-symmetric. Hence, the twisted Frobenius–Schur indicator in these two cases is $+1$ or -1, respectively. Moreover, if the indicator is ± 1, then $U_i^* U_i$ is $\pm\mathbb{1}$; otherwise $\mathrm{tr}\left(U_i^* U_i\right)$ could not be $\pm \dim \boldsymbol{R}_i$. This then implies that U_i is symmetric or anti-symmetric, respectively, and, therefore, that τ is an involution.

Thus, one can conclude that an automorphism is a Bickerstaff–Damhus automorphism if and only if the twisted Frobenius–Schur indicator is $+1$ for all irreducible representations $\boldsymbol{R}_i$ of G. If it is ± 1 for all irreducible representations but not $+1$ for all of them, τ is a class-inverting involution. If the twisted Frobenius–Schur indicator is not ± 1 for all irreducible representations, τ is either not class-inverting or not involutory or neither of the two.

In addition, for involutory τ, a zero of the indicator FS_τ for at least one irreducible representation indicates that τ is not class-inverting. However, for higher-order automorphisms, the twisted Frobenius–Schur indicator can vanish even though the automorphism is class-inverting. For such higher-order automorphisms it can therefore be useful to define the extended twisted Frobenius–Schur indicator which again has the property of being ± 1 for class-inverting automorphisms and zero for at least one irreducible representation otherwise. Let $n := \mathrm{ord}\,(\tau)/2$ for even-order automorphisms and $n := \mathrm{ord}\,(\tau)$ for odd-order automorphisms. Then the n-th extended twisted Frobenius–Schur indicator[23] is defined by

$$\mathrm{FS}_\tau^n(\boldsymbol{R}_i) := \frac{(\dim \boldsymbol{R}_i)^{n-1}}{|G|^n} \sum_{g_1,\dots,g_n \in G} \chi_{\boldsymbol{R}_i}(g_1 \tau(g_1) \cdots g_n \tau(g_n))\,. \tag{6.6}$$

This indicator is again ± 1 for all irreducible representations $\boldsymbol{R}_i$ for class-inverting τ and zero for some irreducible representation otherwise. For the proof, which is analogous to the one given for the normal twisted Frobenius–Schur indicator above, see Section A.4.5. Furthermore, in Appendix C, a GAP code is presented which can be used to compute extended twisted Frobenius–Schur indicators.[24]

VII.7 Three classes of discrete groups

Using the information obtained in the preceding sections on proper CP transformations, the Bickerstaff–Damhus automorphism and the (extended) twisted Frobenius–Schur indicator, it is now possible to categorise all discrete groups into three distinct classes.[25]

Type I: The group G has no class-inverting, involutory automorphisms, i.e. for each automorphism there is at least one irreducible representation such that the associated twisted Frobenius–Schur indicator is zero. Thus, it is impossible to define a consistent CP transformation in a generic setting, i.e. CP is generically violated.

Type II: The group G has at least one class-inverting, involutory automorphism.

Type II A: For at least one of these automorphisms, all twisted Frobenius–Schur indicators are $+1$. Hence, this automorphism is a Bickerstaff–Damhus automorphism,

23 For another generalisation of the twisted Frobenius–Schur indicator, cf. [191].

24 Note that for high–order automorphisms such a computation is rather time consuming. From a computational viewpoint it is better directly to check whether an automorphism inverts all conjugacy classes as done by the function `isClassinverting` also presented in Appendix C.

25 In this classification, the possibility of higher-order class-inverting automorphisms that are not equivalent to an involutory automorphism is neglected for the reasons outlined in Section VII.4.2.

and there is a basis for G with real Clebsch–Gordan coefficients. The automorphism also leads to a proper CP transformation, which is identical to the canonical one in the real Clebsch–Gordan basis.

Type II B: There is no automorphism for which all twisted Frobenius–Schur indicators are +1. Hence, there is no Bickerstaff–Damhus automorphism, and there is no basis with real Clebsch–Gordan coefficients. Nonetheless, one can define a proper CP transformation using this automorphism. The discrete group is then possibly enlarged by a $\mathbb{Z}_2$ factor.

Note that groups of type II A can have additional class-inverting, involutory automorphisms that are not Bickerstaff–Damhus automorphisms, i.e. they may also have CP transformations of type II B. The group itself is nonetheless categorised as type II A. Moreover, it is possible to build models without physical CP violation even with type I groups if the representation content of a model is restricted. This is explained in more detail in Section VII.8 and illustrated by an example in Section VII.9.3.

The classification of discrete groups is also illustrated in Figure VII.3.

Examples for each of the three types are presented in Table VII.1. Note that probably all non-abelian groups of odd order belong to type I, see the proof in Section A.4.3. The only possible caveat to this statement are class-inverting automorphisms that square to non-inner automorphisms. However, no such example is known to us, and we have checked explicitly with GAP that there is no such case for any group up to order 599.

A list with the number of non-equivalent class-inverting automorphisms for each non-abelian group up to order 100 that cannot be written as a direct product can be found in Appendix D. Moreover, in Appendix C, a GAP routine is shown that can be used to look for Bickerstaff–Damhus and class-inverting automorphisms of a finite group, i.e. to determine into which class the group falls.

VII.8 CP as a symmetry and constraints on couplings

In this section, the implications of proper CP transformations on Lagrangians are discussed in detail. In particular, the types of constraints on couplings for type I, type II A and type II B are determined. A discussion of the effects of CP transformations for type I groups might seem contradictory to the statements made above that in generic setting there is no CP transformation for such groups. However, as is also shown in an explicit example in Section VII.9.3, it is possible to define a CP transformation if the representation content of the model at hand is such that for all present representations the Frobenius–Schur indicators for the given automorphism are ± 1. In this case, all statements about the CP transformation matrices U_i made below are only true for these representations. Note, furthermore, that again, for the reasons presented in Section VII.4.2, only involutory automorphisms are considered.

For the discussion of CP transformations, it is convenient to work in a special basis. As, by assumption, the automorphism u has order two, the matrices U_i for the CP transformation of the irreducible representations $\boldsymbol{R}_i$ are either symmetric or anti-symmetric [189]. Specialising from the general case of normal forms for generalised CP transformations discussed in [24], which is also reviewed in Section A.6.4, to symmetric and anti-symmetric matrices, one obtains the result that one can write the U_i as

$$U_i = S_i \, \Sigma_{a/s} \, S_i^T \,, \tag{8.1}$$

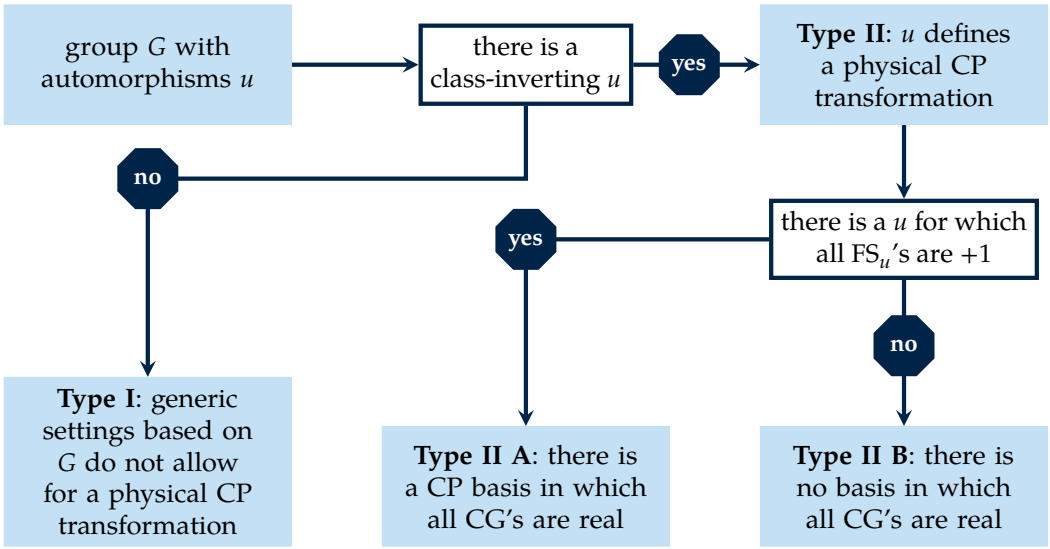


Figure VII.3: The classification of discrete groups into three classes.

G	$\mathbb{Z}_5 \rtimes \mathbb{Z}_4$	T_7	$\Delta(27)$	$\mathbb{Z}_9 \rtimes \mathbb{Z}_3$
SG	(20,3)	(21,1)	(27,3)	(27,4)

(a) Type I.

G	Q_8	A_4	$\mathbb{Z}_3 \rtimes \mathbb{Z}_8$	T′	S_4	A_5
SG	(8,4)	(12,3)	(24,1)	(24,3)	(24,12)	(60,5)

(b) Type II A.

G	$\Sigma(72)$	$((\mathbb{Z}_3 \times \mathbb{Z}_3) \rtimes \mathbb{Z}_4) \rtimes \mathbb{Z}_4$
SG	(72,41)	(144,120)

(c) Type II B.

Table VII.1: Examples for each of the three classes of discrete groups. See (a) for type I, (b) for type II A and (c) for type II B. For each group its trivial name and its SmallGroups library ID are shown.

with unitary S_i and

$$\Sigma_s := \mathbb{1}\,, \qquad \text{if } U_i \text{ is symmetric, i.e. for } \mathrm{FS}_u(\boldsymbol{R}_i) = 1, \tag{8.2a}$$

$$\Sigma_a := \left(\begin{array}{c|c|c} & 1 & \\ -1 & & \\ \hline & \ddots & \\ \hline & & 1 \\ & & -1 \end{array}\right), \qquad \text{if } U_i \text{ is anti-symmetric, i.e. for } \mathrm{FS}_u(\boldsymbol{R}_i) = -1. \tag{8.2b}$$

Note that the anti-symmetric case does not arise for odd-dimensional irreducible representations [189] because the U_i are unitary and, therefore, have full rank. Changing basis to

$$\rho_{\boldsymbol{R}_i}(g) \to S_i^\dagger\, \rho_{\boldsymbol{R}_i}(g)\, S_i\,, \qquad \forall\, g \in G\,, \tag{8.3}$$

the transformed U_i are

$$S_i^\dagger\, U_i\, S_i^* = \Sigma_i = \Sigma_{a/s}\,. \tag{8.4}$$

Before discussing the most general case of contractions of n fields, focus first on the contraction of two fields. Let φ and ψ be two scalar fields transforming in irreducible representations $\boldsymbol{R}_\varphi$ and $\boldsymbol{R}_\psi$ of a discrete group G and consider their contraction to a representation $\boldsymbol{R}_m$, which can be written

$$(\varphi \otimes \psi)_{\boldsymbol{R}_m} = P_{\boldsymbol{R}_m}\, C^\dagger_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi}\, (\varphi \otimes \psi)\,. \tag{8.5}$$

For the definition of the Clebsch–Gordan matrices, see (II.6.6), and note that they are chosen unitary here. The matrix $P_{\boldsymbol{R}_m}$ is the (usually non-diagonal) projection matrix containing only ones and zeros such that

$$P_{\boldsymbol{R}_m} \left(\bigoplus_k \rho_{\boldsymbol{R}_k}(g) \right) P^T_{\boldsymbol{R}_m} = \rho_{\boldsymbol{R}_m}(g)\,, \qquad \forall\, g \in G\,, \tag{8.6}$$

i.e. the projection matrix which singles out the correct representation from the direct sum.

The generalised CP transformation acts on the fields φ and ψ of the contraction (8.5) as

$$\varphi \overset{CP}{\longmapsto} U_{\boldsymbol{R}_\varphi}\, \varphi^*\,, \tag{8.7a}$$

$$\psi \overset{CP}{\longmapsto} U_{\boldsymbol{R}_\psi}\, \psi^* \tag{8.7b}$$

with unitary matrices $U_{\boldsymbol{R}_\varphi}$ and $U_{\boldsymbol{R}_\psi}$.

Note that there are several undetermined phases in these expressions.

(i) As explained in Section II.6, there are adjustable phases in the unitary Clebsch–Gordan matrix $C_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi}$. To be precise, there is one global phase for each irreducible representation $\boldsymbol{R}_k$ in the product of $\boldsymbol{R}_\varphi$ and $\boldsymbol{R}_\psi$.

(ii) The overall phase of each CP transformation matrix U_i can be chosen individually for each field because it is not fixed by equation (4.24). This just reflects the general freedom to re-phase each field operator.

It is now possible to determine the CP transformation behaviour of the compound expression $(\varphi \otimes \psi)_{\boldsymbol{R}_m}$ from the transformations of φ and ψ, [26]

$$\begin{aligned}(\varphi \otimes \psi)_{\boldsymbol{R}_m} &\overset{CP}{\longmapsto} P_{\boldsymbol{R}_m} C^{\dagger}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} \left(U_{\boldsymbol{R}_\varphi} \otimes U_{\boldsymbol{R}_\psi}\right) (\varphi^* \otimes \psi^*) \\ &= P_{\boldsymbol{R}_m} \left[C^{\dagger}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} \left(U_{\boldsymbol{R}_\varphi} \otimes U_{\boldsymbol{R}_\psi}\right) C^{*}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi}\right] C^{T}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} (\varphi^* \otimes \psi^*) \\ &=: P_{\boldsymbol{R}_m} U_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} C^{T}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} (\varphi^* \otimes \psi^*) \,.\end{aligned} \tag{8.8}$$

For type II groups, also the representation $\boldsymbol{R}_m$ has a definite transformation behaviour under CP given by the matrix $U_{\boldsymbol{R}_m}$. One might thus expect that the compound expression $(\varphi \otimes \psi)_{\boldsymbol{R}_m}$ transforms as

$$(\varphi \otimes \psi)_{\boldsymbol{R}_m} \overset{CP}{\longmapsto} U_{\boldsymbol{R}_m} \left[(\varphi \otimes \psi)_{\boldsymbol{R}_m}\right]^* . \tag{8.9}$$

The two transformations are consistent if

$$U_{\boldsymbol{R}_m} P_{\boldsymbol{R}_m} = P_{\boldsymbol{R}_m} U_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} = P_{\boldsymbol{R}_m} C^{\dagger}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} \left(U_{\boldsymbol{R}_\varphi} \otimes U_{\boldsymbol{R}_\psi}\right) C^{*}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} \tag{8.10}$$

up to the aforementioned phases.

Let us discuss this condition for type II A and type II B groups (for type I, see further below).

In the case of type II A groups and if the automorphism that underlies the CP transformation is a Bickerstaff–Damhus automorphism, one can just work in the special basis described above, where the U_i for all irreducible representations $\boldsymbol{R}_i$ are unit matrices. As explained in Section VII.5, this is, for a suitable choice of the free phases, also the basis with real Clebsch–Gordan coefficients. Hence, the condition (8.10) is fulfilled. Moreover, the basis transformation behaviour of the objects in equation (8.10) is such that this holds in any other basis as well for appropriate phase choices.

In the case of type II B groups or if the automorphism that underlies the CP transformation for a type II A group is not a Bickerstaff–Damhus automorphism, the discussion is more involved. There is no basis with completely real Clebsch–Gordan coefficients and not all of the U_i can be transformed to unit matrices, but some of them have instead the anti–symmetric standard form Σ_a. Consider, as an example, the special case where $U_{\boldsymbol{R}_\varphi} = U_{\boldsymbol{R}_\psi} = \mathbb{1}$ and $U_{\boldsymbol{R}_m} = \Sigma_a$. Multiplying equation (8.10) with $P^T_{\boldsymbol{R}_m}$ from the right, one obtains the condition

$$\Sigma_a = P_{\boldsymbol{R}_m} C^{\dagger}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} C^{*}_{\boldsymbol{R}_\varphi \otimes \boldsymbol{R}_\psi} P^T_{\boldsymbol{R}_m} , \tag{8.11}$$

which cannot be true as the right-hand side is a symmetric matrix while the left-hand side is an anti-symmetric matrix. That is, there are cases in which equation (8.10) cannot be solved. Imposing CP as a symmetry removes these problematic terms from the Lagrangian. As we shall see below, this is the extra $\mathbb{Z}_2$ factor described in Section VII.4.2 by which the symmetry group is enlarged.

Let us discuss this again in a more general manner. Note that the only assumptions are that the automorphism chosen is of order two and that only fields in those representations are part of the model that are sent to their conjugates by the automorphism. This covers types II A and II B as well as type I with a restricted representation content.

26 Note that the resulting representation is $\boldsymbol{R}_m \circ u$ instead of $\boldsymbol{R}_m$ because the projection still projects out the same lines as before which now contain, however, the CP transformed representation.

Consider the tensor product $\bigotimes_i \varphi_i$ of fields φ_i in irreducible representations $\boldsymbol{R}_{\varphi_i}$. The corresponding Clebsch–Gordan coefficients are denoted by $C_{\otimes_i \boldsymbol{R}_{\varphi_i}}$ and they fulfil

$$C^\dagger_{\otimes_i \boldsymbol{R}_{\varphi_i}} \left(\bigotimes_i \rho_{\boldsymbol{R}_{\varphi_i}}(g) \right) C_{\otimes_i \boldsymbol{R}_{\varphi_i}} = \bigoplus_k \left(\mathbb{1}_{\mu(k)} \otimes \rho_{\boldsymbol{R}_k}(g) \right) , \quad \forall\, g \in G , \tag{8.12}$$

where $\mu(k)$ is the multiplicity of the irreducible representation $\boldsymbol{R}_k$ in the tensor product. This is just a generalisation of equation (II.6.6) to multiple fields. As can be easily verified, the CP transformation matrix

$$U_{\otimes_i \boldsymbol{R}_{\varphi_i}} := C^\dagger_{\otimes_i \boldsymbol{R}_{\varphi_i}} \bigotimes_i U_{\boldsymbol{R}_{\varphi_i}} C^*_{\otimes_i \boldsymbol{R}_{\varphi_i}} \tag{8.13}$$

that follows from the CP transformations of the individual fields fulfils the consistency equation

$$\bigoplus_k \left(\mathbb{1}_{\mu(k)} \otimes \rho_{\boldsymbol{R}_k}(u(g)) \right) = U_{\otimes_i \boldsymbol{R}_{\varphi_i}} \left(\bigoplus_k \left(\mathbb{1}_{\mu(k)} \otimes \rho_{\boldsymbol{R}_k}(g)^* \right) \right) U^\dagger_{\otimes_i \boldsymbol{R}_{\varphi_i}} , \quad \forall\, g \in G , \tag{8.14}$$

which is just the tensor product version of (4.24). This, by Schur's lemma, implies for type II

$$U_{\otimes_i \boldsymbol{R}_{\varphi_i}} = \left(\bigoplus_k \left(W_k \otimes \mathbb{1}_{\dim(\boldsymbol{R}_k)} \right) \right) \otimes \left(\bigoplus_k \left(\mathbb{1}_{\mu(k)} \otimes U_{\boldsymbol{R}_k} \right) \right) = \left(\bigoplus_k \left(W_k \otimes U_{\boldsymbol{R}_k} \right) \right) \tag{8.15}$$

where the W_k are unitary matrices of dimensions $\mu(k)$.[27] The matrices W_k comprise the unitary transformations between equivalent irreducible representations in the tensor product that are allowed by Schur's lemma. Type I is slightly more complicated and is dealt with further below.

The symmetry or anti-symmetry of the full CP matrix $U_{\otimes_i \boldsymbol{R}_{\varphi_i}}$ follows directly from the symmetry or anti-symmetry of the $U_{\boldsymbol{R}_{\varphi_i}}$ as can be seen from its definition (8.13). If all $U_{\boldsymbol{R}_{\varphi_i}}$ are symmetric, i.e. for type II A, also the matrix $U_{\otimes_i \boldsymbol{R}_{\varphi_i}}$ is symmetric. For type II B, $U_{\otimes_i \boldsymbol{R}_{\varphi_i}}$ is symmetric if an even number of fields of the contraction is in representations with a negative twisted Frobenius–Schur indicator and anti-symmetric if their number is odd.

Since we are only interested in contractions that can be part of a Lagrangian, let us specialise to trivial singlet contractions. In general, a term in the Lagrangian can be written

$$\underline{c}^T P_{(\otimes_i \boldsymbol{R}_{\varphi_i} \to \mathbf{1}_0)} C^\dagger_{\otimes_i \boldsymbol{R}_{\varphi_i}} \bigotimes_i \varphi_i , \tag{8.16}$$

where $\underline{c}$ is an a priori complex coupling vector of the length $\mu(0)$, i.e. of the number of trivial singlets in the contraction. The notation for the projector has been changed to emphasise that it does not only depend on the representation that it projects onto but also on the tensor product of fields it is applied to. Moreover, this projection is assumed to act as an identity matrix on the trivial singlet subspace. Other choices would just reshuffle the couplings and unnecessarily complicate the following computations.

If the contraction (8.16) is part of a Lagrangian, also its complex conjugate term must be present to guarantee that the Lagrangian is real. The condition that CP is a symmetry of the Lagrangian means that the CP transformed term and the complex conjugate term must be identical. The resulting equation then reads

$$\underline{c}^T P_{(\otimes_i \boldsymbol{R}_{\varphi_i} \to \mathbf{1}_0)} U_{\otimes_i \boldsymbol{R}_{\varphi_i}} \stackrel{!}{=} (\underline{c}^T)^* P^*_{(\otimes_i \boldsymbol{R}_{\varphi_i} \to \mathbf{1}_0)} , \tag{8.17}$$

27 Compare [14] for the Lie group case.

which is a generalisation of equation (8.10) to several fields but specialised to trivial singlet contractions. For CP conservation, such a condition has to be fulfilled for each contraction in the Lagrangian. Using (8.15), assuming without loss of generality $U_{\mathbf{1}_0} = 1$ (any phase can be absorbed into W_0) and using that on the singlet subspace the projection acts as the identity, one can simplify the condition of CP invariance for the contraction (8.16) to

$$\begin{aligned} & \underline{c}^T W_0 \stackrel{!}{=} (\underline{c}^T)^* \\ \Leftrightarrow \quad & W_0^T \underline{c} \stackrel{!}{=} \underline{c}^* \,. \end{aligned} \tag{8.18}$$

Consider first type II A. From the symmetry of all $U_{\otimes_i \boldsymbol{R}_{\varphi_i}}$ and equation (8.15), one can see that W_0 must be a symmetric matrix and that it can, hence, be written as

$$W_0 = A^T A \tag{8.19}$$

for some unitary matrix A. Condition (8.18) then becomes

$$A\,\underline{c} \in \mathbb{R}^{\mu(0)} \,. \tag{8.20}$$

This removes one half of the degrees of freedom from the a priori complex couplings $\underline{c} \in \mathbb{C}^{\mu(0)}$ and restricts them to a subspace which is isomorphic to $\mathbb{R}^{\mu(0)}$. This is, of course, what one expects from CP. In fact, going to the CP basis, one can easily convince oneself that $W_0 = \mathbb{1}_{\mu(0)}$, i.e. that CP forces all couplings to be real. This is also not changed by pure basis transformations.

Note that adding (possibly field-dependent) phases to the generalised CP transformations computationally just amounts to changing W_0 to a diagonal phase matrix. In this case, the couplings $\underline{c}$ have fixed but non-trivial phases. Physically this corresponds to a simple re-phasing of the fields and does not lead to different physical observations. Therefore, it is clear that CP is automatically conserved if there is enough freedom of re-phasing to render all couplings real. In generic models, however, there can be more couplings with non-trivial phases than fields, in which case the surplus phases can violate CP explicitly. Concerning their CP properties, type II A groups behave thus analogously to continuous groups.

The second case to be considered is type II B. If an even number of fields in the tensor product is in representations with a negative twisted Frobenius–Schur indicator, the discussion proceeds as for type II A and is not repeated. For an odd number, i.e. anti-symmetric $U_{\otimes_i \boldsymbol{R}_{\varphi_i}}$, W_0 is also anti-symmetric and cannot be written as for type II A. Indeed, using the normal form for unitary matrices in Section A.6.4, one can show that there is no non-trivial solution to (8.18). This might seem surprising because, suddenly, CP forbids terms instead of just restricting phases of couplings. However, in this case

$$V_{\otimes_i \boldsymbol{R}_{\varphi_i}} = U_{\otimes_i \boldsymbol{R}_{\varphi_i}} U^*_{\otimes_i \boldsymbol{R}_{\varphi_i}} = U_{\otimes_i \boldsymbol{R}_{\varphi_i}} (-U^\dagger_{\otimes_i \boldsymbol{R}_{\varphi_i}}) = -\mathbb{1} \,. \tag{8.21}$$

Hence, as already shown above in Section VII.4.2, the CP symmetry implies the presence of an additional $\mathbb{Z}_2$ symmetry, which is responsible for the absence of these terms. That is, type II B groups have the unusual property that CP invariance forbids certain couplings rather than just to restrict the phases of the coefficients. This is illustrated with an explicit example in Section VII.9.2.

This discussion shows that it is always possible to define consistent CP transformations for

type II groups.[28] Whether the transformation is a symmetry just depends on the choice of phases of couplings and, for type II B cases, on the absence of the terms from the Lagrangian that are odd under the additional $\mathbb{Z}_2$.

For type I, the situation is somewhat more complex, partly because there is no CP basis. As already explained, one can only consistently implement a CP transformation corresponding to a specific automorphism of the group if just representations with twisted Frobenius–Schur indicators ± 1 are present as elementary fields in the model. In intermediate stages of contractions, there can, however, appear representations for which this is not true. For any such representation $\boldsymbol{r}$, the assumption that the automorphism is order two together with the solvability of (8.14) and again Schur's lemma imply that also a representation $\boldsymbol{r}'$ equivalent to $(\boldsymbol{r} \circ u)^*$ is part of the tensor product, i.e. $\boldsymbol{r}$ and $\boldsymbol{r}'$ always come in pairs. This allows one to combine $\boldsymbol{r}$ and $\boldsymbol{r}'$ in (8.15) to the reducible representation $\boldsymbol{R} := (\boldsymbol{r}, \boldsymbol{r}')$. Then equation (8.15) is also valid for type I with

$$U_{\boldsymbol{R}} = \begin{pmatrix} 0 & U_{\boldsymbol{r}}^T \\ U_{\boldsymbol{r}} & 0 \end{pmatrix}, \tag{8.22}$$

where $U_{\boldsymbol{r}}$ fulfils

$$\rho_{\boldsymbol{r}}(u(g)) = U_{\boldsymbol{r}}\, \rho_{\boldsymbol{r}'}(g)\, U_{\boldsymbol{r}}^\dagger . \tag{8.23}$$

With this trick the derivation of equation (8.18) can be repeated in complete analogy to type II. However, contrary to type II, there is no guarantee that W_0 is a diagonal matrix due to the structure of $U_{\boldsymbol{R}}$. Indeed, there are cases in which W_0 is non-diagonal. For example, in $\Delta(54)$, there are two trivial singlets in the tensor product contraction

$$\left[(\overline{\mathbf{3}}_1 \otimes \mathbf{3}_2)_{\mathbf{2}_k} \otimes (\mathbf{2}_2 \otimes \mathbf{2}_1)_{\mathbf{2}_k} \right]_{\mathbf{1}_0} , \tag{8.24}$$

one for $k = 3$ and one for $k = 4$.[29] For a convenient choice of basis, the resulting matrix W_0 turns out to be

$$W_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{8.25}$$

such that one coupling is forced to be equal to the conjugate of the other coupling in the CP invariant case. The total number of degrees of freedom of the couplings is still reduced by a factor of two due to the CP symmetry, but their global and relative phases are not fixed.

It is, thus, possible to impose a CP transformation as a symmetry also in type I cases if one restricts the representation content accordingly. However, the constraints put on the couplings by this symmetry are not as simple as in the type II case.

28 Note that the discussion above can also be understood as one direction of a physicists proof of the theorem by Bickerstaff and Damhus [164]. It was shown that given a Bickerstaff–Damhus automorphism, one can transform to a basis in which a given scalar Lagrangian has real couplings and is invariant under the canonical CP transformation, i.e. under complex conjugation of just the fields. For this to be possible, the CP conjugate of each term has to be the same as its complex conjugate. Since the couplings are real, the only difference between the two maps is that in the latter case the Clebsch–Gordan coefficients are conjugated as well. As this difference cannot be counteracted by anything else, the Clebsch–Gordan coefficients must be real.

29 For the $\Delta(54)$ conventions employed, see Section A.1.4.

	$\mathbf{1}_0$	$\mathbf{1}_1$	$\mathbf{1}_2$	$\mathbf{2}_0$	$\mathbf{2}_1$	$\mathbf{2}_2$	$\mathbf{3}$
FS_u	1	1	1	1	1	1	1

Table VII.2: The twisted Frobenius–Schur indicators for the order two representative (9.1) of the non-trivial class of the outer automorphism group of T′.

VII.9 Examples

After the theoretical discussion of the effects of generalised CP transformations, their implications are now illustrated for three example groups. The first example is the double covering of the tetrahedral group T′, which is a type II A group. The example for the slightly more complicated case of type II B is the ambivalent group $\Sigma(72)$. Finally, the example chosen for a type I group is $\Delta(27)$. Information on these three groups can be found in Section A.1.

VII.9.1 Example for type II A: T′

The structure of the automorphism group of T′ has been discussed already in [15]. The outer automorphism group $\mathrm{Out}(\mathrm{T}')$ turns out to be just $\mathbb{Z}_2$. A representative of the non-trivial equivalence class, i.e. the class not containing the identity automorphism, is [15][30]

$$u: \quad (s,t) \quad \mapsto \quad (s^2, t^3) \ . \tag{9.1}$$

This automorphism is an involution and, furthermore, class-inverting, as can be seen from the twisted Frobenius–Schur indicators shown in Table VII.2.

As T′ is not ambivalent, see the characters shown in Table A.2, the identity automorphism is not class-inverting. Thus, the automorphism u of (9.1) is the only automorphism of T′ that can be used for a consistent CP transformation, up to the usual possibility to compose it with an inner automorphism. It is for this reason that Holthausen, Lindner and Schmidt [15] claim to have obtained the unique CP transformation as

$$\mathbf{1}_i \overset{CP}{\longmapsto} \omega^i \, \mathbf{1}_i{}^* \,, \qquad i = 0,1,2 \,, \tag{9.2a}$$

$$\mathbf{2}_i \overset{CP}{\longmapsto} \mathrm{diag}(\psi^{-5}, \psi^5) \, \mathbf{2}_i{}^* \,, \qquad i = 0,1,2 \,, \tag{9.2b}$$

$$\mathbf{3} \overset{CP}{\longmapsto} \mathrm{diag}(1, \omega, \omega^2) \, \mathbf{3}^* \,, \tag{9.2c}$$

where $\omega := \mathrm{e}^{2\pi\,\mathrm{i}\,/3}$, as usual, and $\psi := \mathrm{e}^{\pi\,\mathrm{i}\,/12}$ and where the T′ basis by Feruglio et al. [26, Appendix A] is used, see again also Section A.1.2. This neglects, however, the freedom to change the overall phases of the CP transformation matrices, which are not determined by the consistency condition (4.24). As already mentioned, this choice can, in principle, be made for each field individually and just reflects the unobservability of phase changes of field operators in a quantum field theory. However, it is probably best in most cases not to make use of this freedom once for each field but only once for each irreducible representation. This general freedom to choose phases notwithstanding, the specific choice shown in equation (9.2) seems rather inconvenient.

This can be understood by looking at the contraction of a scalar ψ in representation $\mathbf{2}_0$ with another scalar χ in $\mathbf{2}_1$ to the non-trivial singlet $\mathbf{1}_1$, which, in the basis from [26] is

$$(\psi \otimes \chi)_{\mathbf{1}_1} = \frac{-1}{\sqrt{2}} \, (\psi_1 \chi_2 - \psi_2 \chi_1) \ . \tag{9.3}$$

30 For the group theory of T′ and the notation employed here, see Section A.1.2.

This compound expression does not pick up a phase under the transformation shown in (9.2), although a $\mathbf{1}_1$ is supposed to be multiplied by a factor of ω. Although this is not inconsistent, it is more difficult to do computations with such a choice. Moreover, as shown in Section VII.8, this complication is unnecessary for type II A groups, where one can always choose the phases such that compounds transform like elementary fields.

Indeed, as for any type II A group, one can go to a basis for T′ in which the CP transformation is just the canonical one, i.e. just conjugation of the fields,

$$\mathbf{1}_i \xmapsto{CP} \mathbf{1}_i{}^*\,, \qquad i = 0,1,2\,, \tag{9.4a}$$

$$\mathbf{2}_i \xmapsto{CP} \mathbf{2}_i{}^*\,, \qquad i = 0,1,2\,, \tag{9.4b}$$

$$\mathbf{3} \xmapsto{CP} \mathbf{3}^*\,. \tag{9.4c}$$

The corresponding basis, which is a special case of one of the bases compiled by Ishimori et al. [57], is displayed in Section A.1.2. The Clebsch–Gordan coefficients in this basis are, of course, real.

Transforming from the basis with real Clebsch–Gordan coefficients to the basis used by [26], one obtains the CP transformation

$$\mathbf{1}_i \xmapsto{CP} \mathbf{1}_i{}^*\,, \qquad i = 0,1,2\,, \tag{9.5a}$$

$$\mathbf{2}_i \xmapsto{CP} \mathrm{diag}(1, \mathrm{e}^{5\pi\,\mathrm{i}\,/6})\,\mathbf{2}_i{}^*\,, \qquad i = 0,1,2\,, \tag{9.5b}$$

$$\mathbf{3} \xmapsto{CP} \mathrm{diag}(1, \omega, \omega^2)\,\mathbf{3}^*\,. \tag{9.5c}$$

With this CP transformation and the phases of the Clebsch–Gordan coefficients obtained from the same basis transformation, see Section A.1.2, all compounds transform like elementary fields, thereby simplifying computations compared to the choice (9.2).

However, both the basis with real Clebsch–Gordan coefficients and this modified Feruglio basis suffer from a deficiency related to the triplet representation. The triplet representation is real, and, in principle, there could be real fields in this representation. However, the representation matrices in the real Clebsch–Gordan basis and in the Feruglio basis are not manifestly real. That is, if a real field undergoes such a transformation, it is not real any more but has developed an imaginary part. This is, of course, inconsistent. One, and arguably the best, way to deal with this issue is to go to a basis where the triplet representation matrices are manifestly real. Such a basis is the one by Ma and Rajasekaran [192], which is also shown in Section A.1.2. In this basis, the CP transformation is not the canonical one but rather

$$\mathbf{1}_i \xmapsto{CP} \mathbf{1}_i{}^*\,, \qquad i = 0,1,2\,, \tag{9.6a}$$

$$\mathbf{2}_i \xmapsto{CP} \mathbf{2}_i{}^*\,, \qquad i = 0,1,2\,, \tag{9.6b}$$

$$\mathbf{3} \xmapsto{CP} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \mathbf{3}^*\,. \tag{9.6c}$$

Another way to deal with the problem is outlined in Section A.2. Hence, one can choose between two mutually exclusive options. Either one works in a basis with real Clebsch–Gordan coefficients and a canonical CP transformation. In this case, one has to treat real scalar fields very carefully. Alternatively, one can work in a basis with complex Clebsch–Gordan coefficients and the non-trivial CP transformation shown in (9.6). This removes any issues with real scalar fields. Which basis is more convenient depends on the precise problem

	$\mathbf{1}_0$	$\mathbf{1}_1$	$\mathbf{1}_2$	$\mathbf{1}_3$	$\mathbf{2}$	$\mathbf{8}$
$\mathrm{FS}_{\mathrm{id}}$	1	1	1	1	-1	1

Table VII.3: The twisted Frobenius–Schur indicators for the identity automorphism of $\Sigma(72)$.

to be solved and on the model at hand, e.g. there are no real scalar fields in supersymmetric models.

As the CP transformation is just the canonical one in a suitably chosen basis, see equation (9.4), no explicit T′ model is presented here. CP can be imposed as a symmetry on any T′ model independently of the field content. If there are enough fields to absorb all phases of couplings, CP symmetry is even automatic. If this is not the case, CP can be explicitly broken by these phases. The CP behaviour is thus precisely the same as known from $\mathrm{SU}(N)$ groups like, for example, in the Standard Model and therefore not discussed in more detail.

VII.9.2 Example for type II B: $\Sigma(72)$

The group chosen as an example of the more exotic type II B is $\Sigma(72)$ [189], whose group theory details are presented in Section A.1.5. This group is ambivalent, i.e. inner automorphisms are class-inverting, as can be seen from the fact that all characters are real, see Table A.6. Thus, $\Sigma(72)$ is a type II group.

It turns out that inner automorphisms are the only class-inverting automorphisms of $\Sigma(72)$, and it is most convenient to choose the identity automorphisms as representative. However, by computing the twisted Frobenius–Schur indicators, see Table VII.3, one can easily verify that the identity automorphism is not a Bickerstaff–Damhus automorphism. The group $\Sigma(72)$ is thus of type II B, and there is no basis with completely real Clebsch–Gordan coefficients.

The problematic representation is the doublet $\mathbf{2}$. The simplest CP transformation behaviour one can achieve is

$$\mathbf{1}_i \xmapsto{CP} \mathbf{1}_i{}^*\,, \qquad i = 0,\,1,\,2,\,3\,, \tag{9.7a}$$

$$\mathbf{2} \xmapsto{CP} U_{\mathbf{2}}\,\mathbf{2}^* := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \mathbf{2}^*\,, \tag{9.7b}$$

$$\mathbf{8} \xmapsto{CP} \mathbf{8}^*\,. \tag{9.7c}$$

This is realised in the basis shown in Section A.1.5.

Imposing this CP transformation as a symmetry leads to an enlarged discrete symmetry as described in Section VII.4.2 and Section VII.8. In fact, it is enlarged to $\Sigma(72) \times \mathbb{Z}_2$. The transformation behaviour of irreducible $\Sigma(72)$ representations $\boldsymbol{R}_i$ under the additional $\mathbb{Z}_2$ can be obtained from applying CP twice. Only the doublet transforms non-trivially,

$$V_{\boldsymbol{R}_i} := U_{\boldsymbol{R}_i}\,U^*_{\boldsymbol{R}_i} = \mathbb{1}\,, \qquad \boldsymbol{R}_i \ncong \mathbf{2}\,, \tag{9.8a}$$

$$V_{\mathbf{2}} := U_{\mathbf{2}}\,U^*_{\mathbf{2}} = -\mathbb{1}\,, \tag{9.8b}$$

where $V_{\boldsymbol{R}}$ is the representation matrix of the generator of the additional $\mathbb{Z}_2$ in representation $\boldsymbol{R}$. Hence, this additional $\mathbb{Z}_2$ forbids all terms which contain an odd number of fields in the

	S	X	Y	Ψ	Σ
$\Delta(27)$	$\mathbf{1}_0$	$\mathbf{1}_1$	$\mathbf{1}_3$	$\mathbf{3}$	$\mathbf{3}$
U(1)	$q_\Psi - q_\Sigma$	$q_\Psi - q_\Sigma$	0	q_Ψ	q_Σ

Table VII.4: Field content of the $\Delta(27)$ example model with $\Delta(27)$ representations and U(1) charges. Note that $q_\Psi \neq q_\Sigma$ is assumed to make the two fields distinguishable.

two-dimensional representation **2**. An example of such a term is

$$[\mathbf{2} \otimes (\mathbf{8} \otimes \mathbf{8})_{\mathbf{2}}]_{\mathbf{1}_0} \,. \tag{9.9}$$

It is impossible to write down a CP invariant Lagrangian containing this term.

As seen in Section VII.8, apart from this complication, the discussion of CP transformations can proceed as for type II A. No explicit example model is therefore discussed here.

VII.9.3 Example for type I: $\Delta(27)$

In a sense the most interesting groups are the ones classified as type I. In these groups, CP is, in generic models, broken in the same ways as parity in the Standard Model, i.e. it is broken because one cannot even consistently define such an operation. The reason is, as explained in detail in the preceding sections, that there is no class-inverting automorphism. This shall be illustrated in this section by an example using the group $\Delta(27)$. Moreover, the example gives us an opportunity to comment on the assumption that a model is generic. For the group theory of $\Delta(27)$, see Section A.1.3.

A toy example with CP violation

The toy model to be considered here consists of three scalar fields X, Y and S in the $\Delta(27)$ singlet representations $\mathbf{1}_1$, $\mathbf{1}_3$ and $\mathbf{1}_0$, respectively, and two Dirac spinors Ψ and Σ transforming as $\Delta(27)$ triplets **3**. Moreover, suppose that there is a U(1) symmetry that allows one to distinguish between Ψ and Σ because their charges q_Ψ and q_Σ are different. The scalar fields S and X both have charge $q_\Psi - q_\Sigma$, whereas Y is uncharged. The whole field content is also summarised in Table VII.4.

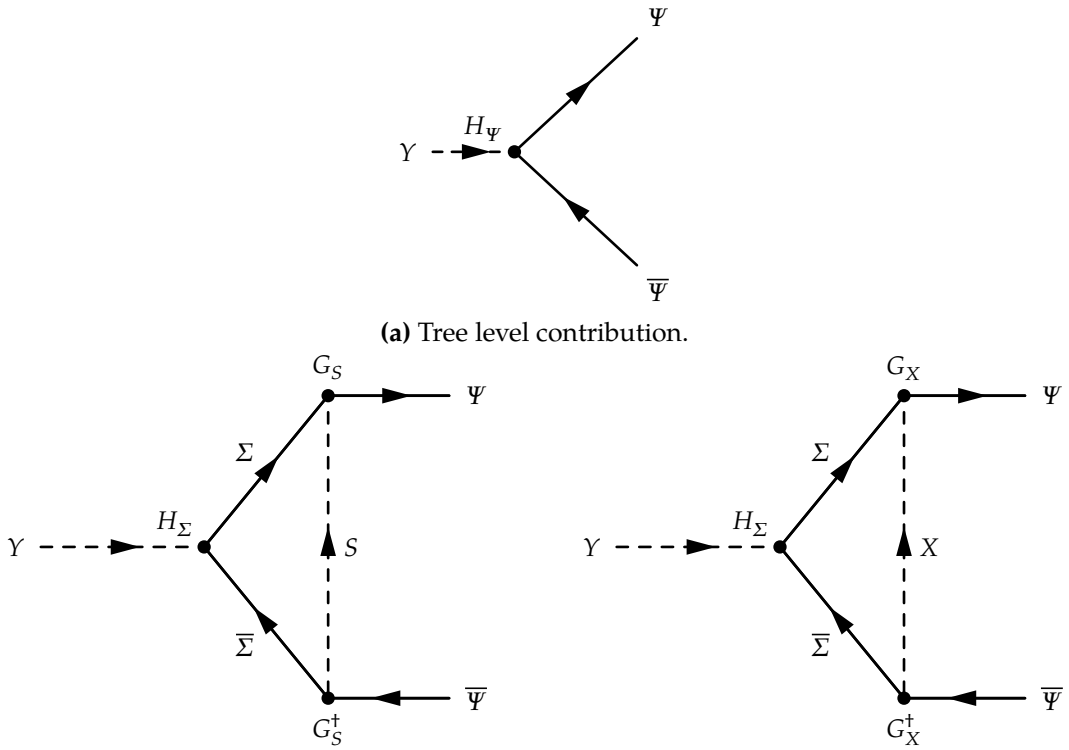
Restricting the Lagrangian to renormalisable terms and imposing all symmetries, the interaction terms of the Lagrangian are

$$\begin{aligned}\mathcal{L} \supset\; & g_S \left[S_{\mathbf{1}_0} \otimes \left(\overline{\Psi} \otimes \Sigma\right)_{\mathbf{1}_0}\right]_{\mathbf{1}_0} + g_X \left[X_{\mathbf{1}_1} \otimes \left(\overline{\Psi} \otimes \Sigma\right)_{\mathbf{1}_2}\right]_{\mathbf{1}_0} + \\ & + h_\Psi \left[Y_{\mathbf{1}_3} \otimes \left(\overline{\Psi} \otimes \Psi\right)_{\mathbf{1}_6}\right]_{\mathbf{1}_0} + h_\Sigma \left[Y_{\mathbf{1}_3} \otimes \left(\overline{\Sigma} \otimes \Sigma\right)_{\mathbf{1}_6}\right]_{\mathbf{1}_0} + \text{h. c.}\,,\end{aligned} \tag{9.10}$$

where $g_{S/X}$ and $h_{\Psi/\Sigma}$ are complex couplings. Note that there is, in principle, also a cubic term in Y, which does, however, not play any role in the following and is thus omitted.

Performing all the contractions using the basis shown in Section A.1.3, the Lagrangian in components is

$$\mathcal{L} \supset (G_S)^{ij}\, S\, \overline{\Psi}_i \Sigma_j + (G_X)^{ij}\, X\, \overline{\Psi}_i \Sigma_j + (H_\Psi)^{ij}\, Y\, \overline{\Psi}_i \Psi_j + (H_\Sigma)^{ij}\, Y\, \overline{\Sigma}_i \Sigma_j + \text{h. c.} \tag{9.11}$$



(a) Tree level contribution.

(b) S loop contribution.

(c) X loop contribution.

Figure VII.4: Feynman diagrams contributing to the decay of the scalar Υ into the Dirac spinor Ψ and its conjugate $\overline{\Psi}$ at tree level, (a) , and one-loop level, (b) and (c).

with the (Yukawa) coupling matrices

$$G_S = g_S \, \mathbb{1} \,, \tag{9.12a}$$

$$G_X = g_X \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} , \tag{9.12b}$$

$$H_{\Psi/\Sigma} = h_{\Psi/\Sigma} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega^2 & 0 \\ 0 & 0 & \omega \end{pmatrix} , \tag{9.12c}$$

where again $\omega := \mathrm{e}^{2\pi \mathrm{i}/3}$.

The CP properties of this toy model shall be discussed by means of the decay asymmetry of the process $\Upsilon \to \overline{\Psi}\Psi$, which can be computed with the formula

$$\varepsilon_{\Upsilon \to \overline{\Psi}\Psi} := \frac{\Gamma(\Upsilon \to \overline{\Psi}\Psi) - \Gamma(\Upsilon^* \to \overline{\Psi}\Psi)}{\Gamma(\Upsilon \to \overline{\Psi}\Psi) + \Gamma(\Upsilon^* \to \overline{\Psi}\Psi)} \,. \tag{9.13}$$

The relevant Feynman diagrams for this process at tree and one-loop level are shown in Figure VII.4. The interference of these diagrams generates the decay asymmetry

$$\begin{aligned} \varepsilon_{\Upsilon \to \overline{\Psi}\Psi} &\propto \operatorname{Im}(I_S) \operatorname{Im}\left[\operatorname{tr}\left(G_S^\dagger H_\Psi G_S H_\Sigma^\dagger\right)\right] + \operatorname{Im}(I_X) \operatorname{Im}\left[\operatorname{tr}\left(G_X^\dagger H_\Psi G_X H_\Sigma^\dagger\right)\right] \\ &= |g_S|^2 \operatorname{Im}(I_S) \operatorname{Im}(h_\Psi h_\Sigma^*) + |g_X|^2 \operatorname{Im}(I_X) \operatorname{Im}(\omega h_\Psi h_\Sigma^*) \,. \end{aligned} \tag{9.14}$$

The abbreviations $I_{S/X}$ denote phase space factors and loop integrals, which depend on the masses of the particles. Note that neither a $\mathrm{U}(1)$ charge nor a left–right asymmetry is produced by the decay. It is, however, possible to distinguish between Y and Y^* by measuring their relative branching fractions to $\overline{\Psi}\Psi$ and $\overline{\Sigma}\Sigma$.

From the expression in terms of traces of the coupling matrices it is clear that, as any physical observable, the decay asymmetry is independent of the $\Delta(27)$ basis used for its formulation. In fact, the traces are basis invariants of the toy model analogous to the ones discussed in Section VII.1.2 for the Standard Model. Moreover, the decay asymmetry is independent of the (unobservable) re-phasing freedom of the fields and does not depend on the phases of g_S and g_X.

It is clear that for CP conservation the decay asymmetry (9.14) would have to vanish. There are two distinct possibilities when this could happen.

The first occurs if the masses of S and X coincide, such that the loop factors are identical, the two couplings g_S and g_X have identical absolute values, and the relative phase of the couplings h_Ψ and h_Σ,

$$\varphi := \arg\left(h_\Psi h_\Sigma^*\right), \tag{9.15}$$

is precisely $\varphi = -2\pi/6$. As one can easily convince oneself, these relations between the couplings cannot be due to a consistent CP transformation. The scalar field S does not transform under $\Delta(27)$ at all, whereas X transforms non-trivially. Therefore, no automorphism of $\Delta(27)$ can lead to a relation between the couplings g_S and g_X or between the masses of S and X. Thus, any symmetry leading to the desired equality of the two absolute values cannot be a CP transformation.

This is in accordance with the fact that $\Delta(27)$ is a type I group. Indeed, for the representations used in the toy model, there is no automorphism of $\Delta(27)$ whose twisted Frobenius–Schur indicators are ± 1 simultaneously for all of them. This is, as can be checked easily with GAP, always the case in $\Delta(27)$ if there is at least one triplet and at least two different, non-conjugate non-trivial singlets.

The second possibility is a tuning of the parameters such that, even if the masses of S and X are different, the decay asymmetry is cancelled due to a special value of φ. Since $\varphi = -2\pi/6$ is the value for equal masses, the respective φ for unequal masses must be different. However, any such value changes non-trivially under the renormalisation group. In fact, the one-loop renormalisation group equation for the product $h_\Psi h_\Sigma^*$ of couplings is

$$16\pi^2 \frac{\mathrm{d}}{\mathrm{d}t}\left(h_\Psi h_\Sigma^*\right) = h_\Psi h_\Sigma^* \times \text{real} + \text{real} \times \left(|h_\Psi|^2 + |h_\Sigma|^2\right)\left(|g_S|^2 + \omega^2 |g_X|^2\right), \tag{9.16}$$

where t is the logarithm of the ratio of the renormalisation scales. Thus, the only phase value that is invariant under the renormalisation group is

$$\varphi = \arg\left(|g_S|^2 + \omega^2 |g_X|^2\right). \tag{9.17}$$

For the aforementioned possibility of equal masses of X and S and equal absolute values of g_X and g_S, this is precisely $\varphi = -2\pi/6$. However, for other values of the couplings, any adjusted phase of $h_\Psi h_\Sigma^*$ runs away from its original value.[31] That is, the assumptions of this second possibility are not invariant under the renormalisation group and receive higher-order quantum corrections. Thus, they cannot be obtained by imposing a symmetry.

31 This has also been checked at two-loop order using pyr@te [193].

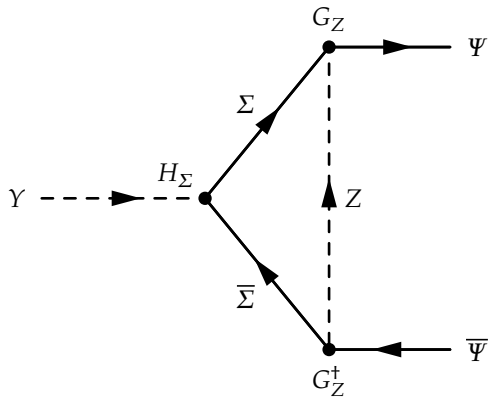


Figure VII.5: Contribution of the Z loop in the modified toy model to the decay asymmetry $\varepsilon_{Y\to\overline{\Psi}\Psi}$.

To conclude, any proper CP transformation, i.e. any transformation mapping each field to its own conjugate, is inconsistent with the $\Delta(27)$ symmetry due to the sufficiently non-generic representation content of the model. Thus, CP is violated in this toy model purely by group theory, somewhat analogous to parity in the SM.

A modified toy model and spontaneous CP violation

Modifying the toy model introduced in the last section, one can build a model with spontaneous CP violation with calculable phases. For spontaneous CP violation, it is, of course, necessary to start with a CP invariant theory in the first place. Since this is, as shown, impossible with the field content shown in Table VII.4, let us exchange the field S with a new scalar field Z with the same $\mathrm{U}(1)$ charge but transforming in $\mathbf{1}_8$ under $\Delta(27)$.

The modified interaction terms of the Lagrangian are

$$\begin{aligned}\mathcal{L} \supset\ & g_Z \left[Z_{\mathbf{1}_8} \otimes \left(\overline{\Psi} \otimes \Sigma\right)_{\mathbf{1}_4}\right]_{\mathbf{1}_0} + g_X \left[X_{\mathbf{1}_1} \otimes \left(\overline{\Psi} \otimes \Sigma\right)_{\mathbf{1}_2}\right]_{\mathbf{1}_0} + \\ & + h_\Psi \left[Y_{\mathbf{1}_3} \otimes \left(\overline{\Psi} \otimes \Psi\right)_{\mathbf{1}_6}\right]_{\mathbf{1}_0} + h_\Sigma \left[Y_{\mathbf{1}_3} \otimes \left(\overline{\Sigma} \otimes \Sigma\right)_{\mathbf{1}_6}\right]_{\mathbf{1}_0} + \text{h. c.}\,,\end{aligned} \tag{9.18}$$

where g_Z is a complex coupling. Writing the new term in component form, one encounters the coupling matrix

$$G_Z = g_Z \begin{pmatrix} 0 & 0 & \omega^2 \\ 1 & 0 & 0 \\ 0 & \omega & 0 \end{pmatrix}. \tag{9.19}$$

The exchange of S with Z implies also that one has to recompute the one-loop contribution to the decay asymmetry $\varepsilon_{Y\to\overline{\Psi}\Psi}$. The Feynman diagram shown in Figure VII.4(c) still contributes but, instead of Figure VII.4(b), there is a new contribution due to Z shown in Figure VII.5.

The decay asymmetry thus changes to

$$\begin{aligned}\varepsilon_{Y\to\overline{\Psi}\Psi} &\propto \operatorname{Im}(I_X)\ \operatorname{Im}\left[\operatorname{tr}\left(G_X^\dagger H_\Psi G_X H_\Sigma^\dagger\right)\right] + \operatorname{Im}(I_X)\ \operatorname{Im}\left[\operatorname{tr}\left(G_X^\dagger H_\Psi G_X H_\Sigma^\dagger\right)\right] \\ &= |g_X|^2\ \operatorname{Im}(I_X)\ \operatorname{Im}\left(\omega\, h_\Psi h_\Sigma^*\right) + |g_Z|^2\ \operatorname{Im}(I_Z)\ \operatorname{Im}\left(\omega^2\, h_\Psi h_\Sigma^*\right).\end{aligned} \tag{9.20}$$

CP is still generically violated because the asymmetry is non-vanishing for generic values of the couplings. It vanishes if the masses of X and Z are identical, the absolute values of g_X and g_Z are the same, and the relative phase of h_Ψ and h_Σ is $\varphi = 0$.

In contrast to the example with the scalar S, this point in parameter space can be understood from a symmetry that is related to an automorphism of $\Delta(27)$. This is possible because Z is, in contrast to S, not a trivial singlet, i.e. it is affected by $\Delta(27)$ automorphisms. A possibility is the non-inner automorphism u_3 defined in (A.1.21). This automorphism can be implemented in the model as

$$X \leftrightarrow Z\,, \tag{9.21a}$$
$$Y \longmapsto Y\,, \tag{9.21b}$$
$$\Psi \longmapsto U_{u_3}\,\Sigma^{CP}\,, \tag{9.21c}$$
$$\Sigma \longmapsto U_{u_3}\,\Psi^{CP}\,, \tag{9.21d}$$

where the matrix U_{u_3} is shown in (A.1.22). This transformation is for the special choice $q_\Psi = -q_\Sigma$ consistent with the U(1) symmetry and ensures all relations necessary for CP invariance. However, the crucial observation is that the transformation (9.21) is not a CP transformation. This is immediately clear from the transformation of the complex scalar Y, which does not transform at all.

To understand why CP is conserved nonetheless, one has to realise that this transformation just enlarges the discrete symmetry of the model, i.e. it is of the type 'proper discrete symmetry' discussed in Section VII.4. This would be even more transparent if one were to relabel Σ^{CP} to, for example, Ξ. The effect of the transformation (9.21) is to enlarge the discrete symmetry to the semi-direct product $\Delta(27) \rtimes_{u_3} \mathbb{Z}_2$. The group structure can be obtained by the methods of [15, 16] or with the help of GAP. In fact, the resulting group is the group SG(54,5) in the SmallGroups library of GAP. In this enlarged symmetry, X and Z are combined into a doublet and Ψ and Σ^{CP} into a hexaplet. Of course, this does still not fully answer the question why CP is conserved after imposing this symmetry. The actual reason is that SG(54,5) is a type II A group, i.e. it has a Bickerstaff–Damhus automorphism, and there are enough re-phasing degrees of freedom from the fields to render all couplings real. That is, in the model with the larger symmetry, CP is automatically, if somewhat accidentally, conserved. Note furthermore that, due to the symmetry, the conditions ensuring CP conservation are renormalisation group invariant, as we have explicitly checked.

The model with a SG(54,5) symmetry is now a candidate model for spontaneous CP breaking because CP is conserved in the beginning. In fact, the group can easily be broken to $\Delta(27)$ because there is a singlet representation which is represented as 1 on the $\Delta(27)$ subgroup and as -1 on all other group elements. A real singlet scalar field with trivial U(1) charge in this representation has, at the renormalisable level, the interactions

$$\mathcal{L} \supset \left[\frac{\mu}{\sqrt{2}}\,\varphi\,\left(|X|^2 - |Z|^2\right) + \text{h. c.}\right] \tag{9.22}$$

with the other fields of the toy model. A non-trivial vacuum expectation value, as obtained from the usual Higgs type potential with quadratic and quartic term (a cubic term is forbidden by SG(54,5)) hence generates a mass splitting between the X and Z fields. However, the other relations among couplings are still valid.

Therefore, after spontaneous breaking, the decay asymmetry is non-vanishing,

$$\varepsilon_{Y\to\overline{\Psi}\Psi} \propto |g_X|^2\,|h_\Psi|^2\,\text{Im}\,(\omega)\,\left[\text{Im}\,(I_X) - \text{Im}\,(I_Z)\right]\,, \tag{9.23}$$

and all phases are completely determined by group theory. They do not depend on any parameters of the model, i.e. they are calculable.

Recipe for spontaneous CP violation with calculable phases

This can actually be seen as a recipe for spontaneous CP violation with calculable phases.

One starts with a model which has as symmetry group a type II group and implements a consistent CP symmetry at this level. Then one breaks this group spontaneously to a type I subgroup. Depending on the emerging representation content, one obtains a CP violating theory.

Note, however, that this does not work in all cases. In fact, in Section VI.4.5, it was shown that breaking $\mathrm{SU}(3)$ to $\Delta(27)$, where $\mathrm{SU}(3)$ can be seen as a continuous type II A group, one can only obtain non-generic representation contents of $\Delta(27)$.[32]

CP-like symmetries

Using the toy model with the scalar Z it is also possible to show that CP-like symmetries do not lead to physical CP conservation. To this end, instead of the automorphism u_3, impose the transformation

$$\varphi \longmapsto \varphi^* \,, \qquad \varphi = X, Y, Z \,, \tag{9.24a}$$

$$\Psi \longmapsto U_{u_5}\, \Sigma \,, \tag{9.24b}$$

$$\Sigma \longmapsto U_{u_5}\, \Psi \,, \tag{9.24c}$$

corresponding to u_5 in (A.1.21) as a symmetry, which is the same as u from [15]. This transformation is consistent with the $\mathrm{U}(1)$ symmetry for the choice $q_\Psi = -q_\Sigma$ and acts on the $\mathrm{U}(1)$ charges like a charge conjugation.

However, it is not a proper CP transformation as it maps **3** to itself in $\Delta(27)$. This is reflected by the fact that the decay asymmetry $\varepsilon_{Y\to\overline{\Psi}\Psi}$ shown in (9.20) does not vanish if (9.24) is imposed as a symmetry.

Summary of the $\Delta(27)$ toy models

After discussing the toy models it should have become clear that, in generic $\Delta(27)$ models, physical CP is violated. This has nothing to do with phases of couplings but is purely a consequence of the group structure of $\Delta(27)$, namely of its automorphisms. Using this knowledge, it was possible to construct a (toy) model of spontaneous CP violation with calculable phases by embedding the $\Delta(27)$ model into a model with a larger type II A symmetry group.

VII.10 Clarification of geometrical CP violation

After presenting the toy model with $\Delta(27)$ symmetry in the previous section, some comments seem appropriate concerning the well-known three Higgs doublet model (3HDM) by Branco, Gerard and Grimus [17], which is constructed to be symmetric under $\Delta(27)$ in addition to the inherent $\mathrm{SU}(2)_\mathrm{L} \times \mathrm{U}(1)_\mathrm{Y}$ of the Higgs doublets. Since it contains only triplets, there are $\Delta(27)$ automorphisms which can be used to implement a consistent CP transformation, e.g.

32 The possibility of this breaking has been discussed in [151].

u_1 of (A.1.21). Note that this is spoilt as soon as two different, non-conjugate non-trivial singlets are introduced. As it turns out, CP in this model is, for certain ranges of coupling values, spontaneously violated in a peculiar way that is called geometrical CP violation. This section tries to clarify some issues related to this effect.

VII.10.1 The three Higgs doublet potential with $\Delta(27)$ symmetry

The Higgs potential of the three Higgs doublet model by Branco, Gerard and Grimus [17] can be written as

$$\begin{aligned} V(H) \coloneqq & -m^2 H_i^\dagger H_i + \lambda_1 \left(H_i^\dagger H_i\right)^2 + \lambda_2 \left(H_i^\dagger H_i\right) \left(H_j^\dagger H_j\right) + \lambda_3 \left(H_i^\dagger H_j\right) \left(H_j^\dagger H_i\right) \\ & + \tilde{\lambda}_4 \left[\left(H_1^\dagger H_2\right) \left(H_1^\dagger H_3\right) + \text{cyclic}\right] + \text{h. c.}\,, \qquad i,j = 1,\,2,\,3 \text{ with } i \neq j\,. \end{aligned} \tag{10.1}$$

It turns out to be convenient to write $\tilde{\lambda}_4$ as a polar decomposition

$$\tilde{\lambda}_4 =: \lambda_4 \, \mathrm{e}^{\mathrm{i}\,\Omega}\,, \qquad \lambda_4 > 0\,, \qquad 0 \leq \Omega < 2\,\pi\,. \tag{10.2}$$

All other couplings are real and assumed to be chosen such that the potential is bounded below.

The original model was introduced by demanding invariance under a $\Delta(27)$ flavour symmetry, with H transforming as a triplet, in addition to the $\mathrm{SU(2)_L} \times \mathrm{U(1)_Y}$ electroweak gauge symmetry. Due to the restriction to renormalisable terms and the additional continuous symmetries, the model is, in fact, invariant under the larger group $\Delta(54)$, under which H transforms as $\mathbf{3}_1$ [161–163, 194].[33] For further information on $\Delta(27)$ and $\Delta(54)$, see Section A.1.3 and Section A.1.4, respectively.

It is furthermore assumed that the global minimum of the potential preserves electric charge, i.e. that it can be parametrised as

$$\langle H_i \rangle = \begin{pmatrix} 0 \\ v_i \, \mathrm{e}^{\mathrm{i}\,\varphi_i} \end{pmatrix}\,, \qquad i = 1,\,2,\,3\,. \tag{10.3}$$

This assumption is, in principle, a non-trivial constraint because, contrary to models with at most two doublets [195, 196], there can be charge-breaking minima in a 3HDM [197]. However, using the equivalence transformations discussed in [4], one can always bring the VEVs into such a form that the arguments of [197] can be used to show that all minima are charge-conserving. Therefore, for VEVs of the Higgs triplet, only the charge-conserving lower components are shown hereafter.

A careful computation reveals that, depending on the couplings, there are four possible types of minima [194, 198],

$$v_{\mathrm{I}} \coloneqq v \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\,, \qquad v_{\mathrm{II}} \coloneqq v \begin{pmatrix} \omega \\ 1 \\ 1 \end{pmatrix}\,, \qquad v_{\mathrm{III}} \coloneqq v \begin{pmatrix} \omega^2 \\ 1 \\ 1 \end{pmatrix}\,, \qquad v_{\mathrm{IV}} \coloneqq v \begin{pmatrix} \sqrt{3} \\ 0 \\ 0 \end{pmatrix}\,, \tag{10.4}$$

where, as always, $\omega \coloneqq \mathrm{e}^{2\pi\,\mathrm{i}\,/3}$ and where v denotes functions that depend on the couplings. A detailed explanation of the minimisation procedure can be found in Appendix B of [4].

33 Simply speaking, under $\Delta(27)$ only cyclic permutations of the triplet components should be a symmetry transformation. However, also transpositions of components are symmetries of the potential, thus enlarging the symmetry group to $\Delta(54)$.

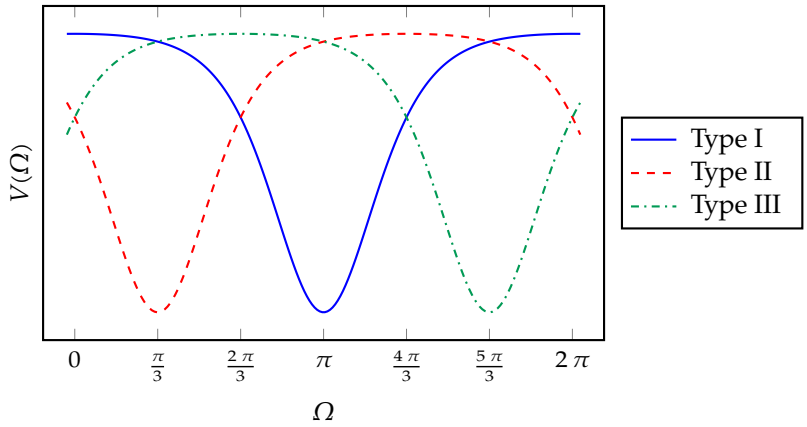


Figure VII.6: For any given value of the phase Ω, one can read off the type of minimum by determining which curve is the lowest. For phases $\Omega \in \{0, 2\pi/3, 4\pi/3\}$, there are two degenerate types of minima. For all other phase values, the type of the global minimum is unique.

Note that any of the four types of vacuum expectation values corresponds to a whole orbit of different VEVs, which can be obtained by acting with all symmetry elements on it. This implies, in particular, that, due to the $\mathrm{U}(1)_\mathrm{Y}$ gauge symmetry, the overall phase of the VEVs is not fixed.

Which of the four types of vacuum expectation values shown in (10.4) is the global minimum of the potential depends on the values of the couplings. One can fix the couplings λ_i in such a way that type IV is excluded. Then the phase Ω alone determines the type of VEV. Figure VII.6 shows the type of the global minimum for this case in dependence of the phase Ω. The parameter space for Ω splits into three different regions with a unique global minimum inside the regions and two degenerate global minima on their borders.

The fact that the relative phases of the VEVs shown in equation (10.4) do not depend continuously on the couplings is called geometrical CP violation [17]. This is now explained in more detail.

VII.10.2 Geometrical CP violation

The 3HDM introduced above is known best for the fact that the model leads to geometrical CP violation [17].[34] In fact, one should rather use the alternative name calculable phases for this effect, which can also be found in the original publication by Branco, Gerard and Grimus [17]. This can be understood as follows.

Contrary to popular beliefs, the main point of geometrical CP violation is not the fact that there are relative phases between the components in the vacuum expectation values of types II and III. Indeed, also the VEVs of types I and IV violate CP geometrically. This becomes immediately clear if one takes into account the possibility of basis transformations. One can always find a unitary rotation that transforms a given triplet VEV to $(1, 0, 0)^T$ and vice versa. That is, one can transform any (single) VEV to one without any relative phases. The phases are then contained in the CP transformation matrix U_{CP}. Alternatively, one can introduce relative phases into any given VEV. The occurrence of relative phases is thus

34 In fact, Branco, Gerard and Grimus [17] discussed geometrical T violation, but, due to CPT invariance, the two notions are equivalent.

connected to the basis in which the computation is performed and, therefore, no physical effect. However, the fact that the phases do not continuously depend on the couplings, i.e. that they are calculable, is highly non-trivial and the proper meaning of the term geometrical CP violation.

To illustrate this further, take the CP transformation

$$H \xmapsto{CP} U_{u_4} H^* \tag{10.5}$$

connected to the automorphism $u_4 : \quad (a, b) \quad \mapsto \quad (ab^2 a, b)$ (see also (A.1.21)), where

$$U_{u_4} := \begin{pmatrix} \omega^2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{10.6}$$

is the solution to the consistency condition (4.24) for the triplet **3**. Note that the automorphism u_4 is not class-inverting, which is clear as $\Delta(27)$ is a type I group. However, only the Higgs triplet in representation **3** is present which is indeed conjugated by u_4.

The CP transformation (10.5) is a symmetry of the Lagrangian for Ω being either $\pi/3$ or $4\pi/3$. Let hence $\Omega = 4\pi/3$. According to Figure VII.6, the VEV can either be of type I or of type III. Both types, however, break the CP transformation (10.5); thus, CP is spontaneously broken in any case and, in fact, both breakings are geometrical. The geometrical phase resides either in both the VEV and the CP transformation matrix U_{u_4} or only in the latter.

This is even more easily understood if one performs a basis change, see equation (3.6), on the Higgs triplet to bring U_{u_4} to canonical form. The necessary basis transformation is

$$V := \begin{pmatrix} -\omega^2 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & \mathrm{i}/\sqrt{2} & -\mathrm{i}/\sqrt{2} \end{pmatrix} . \tag{10.7}$$

In this case, the geometrical phases are completely contained in the basis-transformed VEVs of type I and III,

$$v'_{\mathrm{I}} := v \begin{pmatrix} -\omega^2 \\ \sqrt{2} \\ 0 \end{pmatrix} , \qquad v'_{\mathrm{III}} := v \begin{pmatrix} -\omega \\ \sqrt{2} \\ 0 \end{pmatrix} , \tag{10.8}$$

while $U'_{u_4} = \mathbb{1}$. From this it is easy to see that it is impossible to go to a basis where the CP transformation matrix and the VEV components are real simultaneously.

To summarise, geometrical CP violation is not signalled by just some relative phases between the individual components of a single vacuum expectation value because this is clearly basis-dependent. Rather, it is an interplay between the relative phases of the VEV and the CP transformation. Only if the phases do not depend continuously on the couplings, one should consider a spontaneous CP violation geometrical.

VII.11 The strong CP problem and generalised CP transformations

Besides the weak Dirac CP phase δ_{CP} there is one more possible source of CP violation in the Standard Model. This is the θ_{QCD} term of QCD, i.e. the term

$$\mathcal{L} \supset \theta_{\mathrm{QCD}} \frac{g_s^2}{32\,\pi^2} F_{\mu\nu,a} \tilde{F}_a^{\mu\nu} , \tag{11.1}$$

where, as in Chapter IV, $\tilde{F}^{\mu\nu} := \frac{1}{2}\,\varepsilon^{\mu\nu\rho\sigma}\,F_{\rho\sigma}$ is the dual field strength tensor. Note that θ_{QCD} is a combination of a bare parameter and of phases from the quark mass matrices,

$$\theta_{\text{QCD}} := \theta^0_{\text{QCD}} + \arg\det Y_u\, Y_d\,. \tag{11.2}$$

Measurements of the neutron electric dipole moment constrain $\theta_{\text{QCD}} \lesssim 10^{-10}$ [33], which seems to be an extremely fine-tuned value. This issue is called the strong CP problem of the Standard Model. A spontaneously broken global $\mathrm{U}(1)$ symmetry was proposed by Peccei and Quinn [199] as a solution; however, this leads to the introduction of potentially problematic axions [200, 201]. Another famous solution is the Nelson–Barr proposal [202, 203], in which CP is spontaneously broken in such a way that no tree level contribution arises. However, one has to make sure that quantum corrections to θ_{QCD} [204] do not spoil this result. Working in a supersymmetric set-up may help in this respect due to the non-renormalisation theorems, cf. [205]. For a very recent assessment of these solutions, cf. [206].

Having followed the discussion on proper (and improper) generalised CP transformations, one might thus try to obtain a different solution to the strong CP problem using this framework. Hence, the goal is to force $\theta_{\text{QCD}} = 0$ by a generalised CP symmetry while at the same time allowing for $\delta_{CP} \neq 0$.

VII.11.1 Using a proper generalised CP transformation

The most natural option seems to be a 'proper' generalised CP transformation. That is, the symmetry to be invoked is of the type

$$f \mapsto U_f f^{CP}\,, \qquad f = q,\, u^c,\, d^c\,. \tag{11.3}$$

Here, the quark triplets transform in irreducible or reducible representations of the discrete symmetry group of the model. However, as was the reason for the definition of 'proper' CP transformations, the transformation (11.3) must be broken to generate a non-trivial δ_{CP}. This can again explicitly be seen from the Jarlskog determinant (1.20) as discussed in Section VII.1.2. Thus, any proper CP symmetry can only protect θ_{QCD} down to the scale at which a non-trivial δ_{CP} is generated. Whether together with δ_{CP} also imaginary parts for the determinants of the mass matrices are generated depends on the details of the model and is no longer controlled by the symmetry. Hence, one can only achieve a solution following the Nelson–Barr approach. In conclusion, proper generalised CP transformations, although, of course, necessary to build Nelson–Barr-like models with discrete flavour symmetries, do not provide genuinely new solutions to the strong CP problem of the SM.

VII.11.2 Using a mixed type symmetry in addition to a CP symmetry

Since a proper CP transformation does not open new avenues for a solution to the strong CP problem, one can try to employ the formerly discarded CP-like transformations. That is, assume that in addition to a proper CP transformation that forbids the bare θ^0_{QCD} term and that is broken to generate a non-trivial δ_{CP}, there is a second symmetry that prevents the determinant of the quark matrices from developing an imaginary part. As this second symmetry cannot be a proper CP transformation, it acts on the quark sector either like a normal flavour symmetry or like a mixed-type symmetry, i.e. a symmetry relating some f_i to f_j^{CP} ($f = q,\, u^c,\, d^c$) and some other f_i to a f_j.

As was already mentioned in Section VII.4.1, such a mixed transformation clashes with Standard Model gauge invariance. Indeed, for the quarks with a proper CP transformation behaviour to be able to couple to gluons, the QCD gauge bosons would have to transform as shown in (1.14), i.e. as known from the SM CP transformation. However, then the quarks which transform to themselves (or some other non-conjugated quark) cannot couple to the gluons because their gauge coupling terms are only invariant if the gluons are completely invariant under the transformation.

These considerations together with those of the previous section imply that there is no symmetry solution to the strong CP problem sending any quark to a conjugate quark. Apart from normal discrete flavour symmetries, the only type of transformation that thus remains is the mixed type with all quarks transforming as under a flavour symmetry and only some additional particles, e.g. flavons, transforming as under a CP transformation. However, apart from the general problems with CP-like transformations discussed in Section VII.4.1, such solutions are completely model-dependent. They are therefore not discussed here in any more detail.

VII.11.3 Summary

Unfortunately, one has to conclude that, while knowledge of generalised CP transformations is clearly necessary to build models solving the strong CP problem with a Nelson–Barr-like approach and discrete non-abelian flavour symmetries, these CP transformations do not open up any completely new opportunities. This is true even if one allows for additional CP-like transformations, which can only be such that they act as normal symmetry operations at least on the quark sector of the SM.

VII.12 Spontaneous symmetry breaking and generalised CP transformations

One particularly interesting approach to the quest for an explanation of the experimentally measured CP violation in the Standard Model is spontaneous CP violation [207]. In combination with a discrete flavour symmetry, one would thereby assume that a generalised CP transformation is a symmetry at a high scale and is then broken spontaneously together with the flavour symmetry or at a different stage. The presumably best outcome would be if all CP violating phases were determined by the group theory, i.e. if they did not continuously depend on adjustable couplings. In this way, one could obtain unambiguous predictions for CP violating quantities. This is, for example, the case in the $\Delta(27)$ model by Branco, Gerard and Grimus [17] discussed before.

Note that CP is spontaneously broken if a consistent CP transformation

$$\Phi \xrightarrow{CP} U_{CP}\, \Phi^* \tag{12.1}$$

is a symmetry of the Lagrangian, where Φ contains all scalar fields of the model,[35] but is not respected by the true vacuum of the theory,

$$U_{CP}\, \langle \Phi \rangle^* \neq \langle \Phi \rangle\,. \tag{12.2}$$

35 An analogous transformation for higher-spin particles is understood.

Note that, if the original theory is symmetric under a group G with Φ transforming with representation matrices ρ_Φ, according to the discussion in Section VII.3, not only the transformation (12.1) is a symmetry of the theory but also any CP transformation

$$\Phi \overset{CP'}{\longmapsto} \rho_\Phi(g)\, U_{CP}\, \Phi^* \,, \qquad \forall\, g \in G \,. \tag{12.3}$$

All of these transformations must be broken in order to achieve spontaneous CP violation. Equation (12.2) should thus rather be replaced with the more precise condition

$$U_{CP}\, \langle \Phi \rangle^* \neq \rho_\Phi(g)\, \langle \Phi \rangle \,, \qquad \forall\, g \in G \,. \tag{12.4}$$

Whereas it is clear that CP is broken if the condition (12.4) is fulfilled, it is non-trivial to investigate the case in which the CP transformation is not broken explicitly by the VEV, i.e. (12.4) is not fulfilled, while G is broken spontaneously to a subgroup H.

VII.12.1 Restrictions of automorphisms to subgroups

Since CP transformations are controlled by class-inverting automorphisms, in order to determine the fate of a CP transformation when the discrete group is spontaneously broken, one has to understand the restriction of such automorphisms to subgroups. That is, one has to understand what kind of CP transformations are available after the breaking and whether any of them is a remnant of the original CP transformation, in which case CP stays unbroken.

Given a subgroup H of G and an automorphism τ of G one can consider its restriction to H,

$$\tilde{\tau} := \tau|_h : \quad H \quad \to \quad G \quad . \tag{12.5}$$

It is clear that, as the restriction of an automorphism, $\tilde{\tau}$ is a group homomorphism from H into G and that it is injective. However, this does not imply that $\tilde{\tau}$ is an automorphism of H. In fact, not even $\tilde{\tau}(H) \subseteq H$ is generally true. For $\tilde{\tau}$ to be an automorphism of H, in general, both $\tilde{\tau}(H) \subseteq H$ and $\tilde{\tau}^{-1}(H) \subseteq H$ must hold. For finite groups H it is sufficient that $\tilde{\tau}(H) \subseteq H$ because injectiveness then also implies surjectiveness.

VII.12.2 Class-inverting automorphisms and spontaneous CP violation

As a CP transformation is not just linked to any automorphism but specifically to a class-inverting automorphism u, one has to distinguish, in fact, three possible cases when breaking a group G spontaneously to a discrete subgroup H. In the first case, the restriction of the class-inverting automorphism u to the subgroup is not even an automorphism of the subgroup. Alternatively, the automorphism could also restrict to an automorphism of the subgroup. Then it is either class-inverting also for the subgroup or not class-inverting. These three cases are now considered in turn. In each case, u denotes the class-inverting automorphism of G corresponding to the generalised CP transformation (12.1) under consideration.

Moreover, in all three case, it is, of course, assumed that equation (12.4) is not fulfilled since, otherwise, CP would be broken directly by the VEV.

The restriction of u is not an automorphism of the subgroup

In this case, it can be shown that it is impossible to break G to H without breaking CP simultaneously by the vacuum expectation value.

By assumption, the vacuum expectation value of Φ breaks G to H, i.e.

$$\rho_\Phi(g)\,\langle\Phi\rangle \begin{cases} = \langle\Phi\rangle & g \in H\,, \\ \neq \langle\Phi\rangle & g \notin H\,. \end{cases} \tag{12.6}$$

Moreover, the CP transformation (12.1) fulfils the consistency condition (4.24). Let furthermore

$$U_{CP}\,\langle\Phi\rangle^* = \langle\Phi\rangle\,, \tag{12.7}$$

i.e. assume that CP is not spontaneously broken.

Let $h \in H$ and assume that $u(h) = g$ with $g \in G \setminus H$. Then

$$\rho_\Phi(g)\langle\Phi\rangle \begin{cases} \neq \langle\Phi\rangle \\ = U_{CP}\,\rho_\Phi(h)^*\,U_{CP}^{-1}\,\langle\Phi\rangle = \langle\Phi\rangle\,, \end{cases} \tag{12.8}$$

which is a contradiction. Thus, $u(h) \neq g$ for all $g \in G \setminus H$, i.e. $u(h) \in H$.

Let again $h \in H$ and $g \in G \setminus H$ but with $u^{-1}(h) = g$. Then

$$\rho_\Phi(g)\langle\Phi\rangle \begin{cases} \neq \langle\Phi\rangle \\ = (U_{CP}^{-1})^*\,\rho_\Phi(h)^*\,U_{CP}^{*}\,\langle\Phi\rangle = \langle\Phi\rangle\,, \end{cases} \tag{12.9}$$

is again a contradiction and, hence, $u^{-1}(h) \in H$. Together, $u(H) \subseteq H$ and $u^{-1}(H) \subseteq H$ imply that u is an automorphism of H, which contradicts the assumption.

This shows that if u does not restrict to an automorphism of H, G can only be broken to H if the CP transformation is also broken, i.e. if equation (12.4) holds.

An example for this case is the subgroup SG(63,1) of $\mathrm{U}(3)$, which can be embedded using one of its triplet representations (GAP #12). There is no CP transformation for this triplet because there is no automorphism that relates this representation to its conjugate one. In particular, since there is no automorphism of SG(63,1) that could be the restriction of the CP transformation of $\mathrm{U}(3)$, it is impossible to break $\mathrm{U}(3)$ to SG(63,1) without also spontaneously breaking CP.

Turning the result just obtained around, one can conclude that if G can be spontaneously broken to H either the CP transformation is broken as well, and thus no symmetry of the broken phase, or its restriction to H is again related to an automorphism of H, i.e. one of the remaining two cases is at hand.

The restriction of u is an automorphism of the subgroup that is not class-inverting

Even if u restricts to an automorphism of the subgroup H, one must not assume that it is also class-inverting for the subgroup. Thus, the restriction of the CP transformation might only be a CP-like transformation of H.

This occurs, for example, in the $\Delta(27)$ model discussed in Section VII.9.3, or rather in its SG(54,5) extension. Indeed, the spontaneous breaking of SG(54,5) to $\Delta(27)$ in (9.22) is due

to the vacuum expectation value of a real singlet scalar field. Thus, the CP transformation is certainly not broken by the vacuum expectation value, i.e.

$$U_{CP}\,\langle\Phi\rangle^* = \langle\Phi\rangle \tag{12.10}$$

holds. However, the proper SG(54,5) CP transformation is only a CP-like transformation for the $\Delta(27)$ symmetry that remains after the breaking and, hence, does not guarantee, as seen in equation (9.23), CP invariance. As a matter of fact, the Bickerstaff–Damhus automorphism of SG(54,5) is such that the CP transformation of the hexaplet $\Psi \oplus \Sigma^{CP}$ is schematically

$$\begin{pmatrix} \Psi \\ \Sigma^{CP} \end{pmatrix} \xrightarrow{CP} U_{CP} \begin{pmatrix} \Psi^{CP} \\ \Sigma \end{pmatrix} = \begin{pmatrix} \Sigma \\ \Psi^{CP} \end{pmatrix}, \tag{12.11}$$

i.e. it is just an exchange of Ψ and Σ. On the level of the representations, the restriction of the automorphism to $\Delta(27)$ does not relate the $\Delta(27)$ triplet $\mathbf{3}$ to the anti-triplet $\overline{\mathbf{3}}$ but sends $\mathbf{3}$ to itself. The remnant of the SG(54,5) CP transformation does hence not lead to physical CP conservation on the $\Delta(27)$ level. This phenomenon could be called indirect spontaneous CP violation because the CP transformation itself is not broken; it is rather the mass splitting, here between the scalars X and Z, due to the flavour symmetry breaking that turns a proper CP transformation into a CP-like transformation.

The general lesson one can draw from this example is that some G representations can split up into several inequivalent H representations such that the CP transformation of G is only CP-like for the subgroup H. Another example of this that has been checked is the breaking of SU(3) to $\Delta(27)$, see also the discussion in Section VI.4.5.

Note, however, that it is impossible to generate a Dirac CP phase δ_{CP} for the SM mass matrices with this mechanism for the same reasons that prohibited a solution to the strong CP problem. As the CP-like transformation is unbroken also in the low-energy theory and the remnant of a proper CP transformation, it still prohibits a non-trivial Jarlskog determinant.

The restriction of u is a class-inverting automorphism of the subgroup

This last case is the simplest one, as the CP transformation of G is also a valid CP transformation for H. Hence, CP is unbroken as long as the vacuum expectation value does not break CP directly via (12.4).

VII.12.3 Summary

The fate of a CP symmetry after the spontaneous breaking of a discrete symmetry group is determined by the restriction of the automorphism defining CP to the unbroken subgroup. Fortunately, as shown above, the paradoxical case that a group G is broken to one of its subgroups H in such a way that the CP transformation is unbroken but not related to any automorphism of H cannot actually arise. Instead, on the one hand, the CP transformation can just directly be broken by the VEV, i.e. equation (12.4) can hold. On the other hand, if the CP transformation is not directly broken by the vacuum expectation value, i.e. if $U_{CP}\,\langle\Phi\rangle^* = \langle\Phi\rangle$, it is either completely unbroken or it is indirectly broken to a CP-like symmetry. However, this latter type of breaking does not allow for the generation of a non-trivial δ_{CP} for the SM.

VII.13 CP as inversion of quantum numbers

In Section VII.4.1, physical criteria for CP transformations were collected, i.e. criteria that allow one to decide whether a transformation should be called CP. These criteria were then used to single out automorphisms that lead to proper CP transformations. In their discussion of CP transformations for continuous symmetries, Grimus and Rebelo [14] also do not consider every transformation that is related to an automorphism via the consistency condition (3.3) a CP transformation. In fact, their criterion is that 'CP reverses all quantum numbers of each field' [14], by which they mean that all weights are multiplied with -1. This criterion certainly suits well the interpretation of CP in QED and in the Standard Model. Moreover, it is equivalent to saying that time reversal, which is the missing piece to arrive at CPT, which certainly inverts all weights, should only revert the direction of motion but not affect the characteristics of particles. Note that one can discuss generalised time reversal transformations for which this is not true. These transformations act like the combination CT does in QED, cf. e.g. [165, 168, 180].

It is instructive to check how the condition of inverted quantum numbers can be formulated for discrete groups and how it relates to the condition found in Section VII.4.1, i.e. that the automorphism must be class-inverting. In order to answer these question, one first has to understand how to define quantum numbers for discrete groups.

VII.13.1 Quantum numbers and symmetries

Quantum numbers are eigenvalues of observables, i.e. of self-adjoint operators that commute with the Hamiltonian and that are time-independent. Under these conditions eigenvalues of the observable are conserved quantities and can be used to label states. Note that the states that are created by a field Φ in an interacting quantum field theory are not eigenstates of the Hamiltonian itself, i.e. there are non-trivial scattering processes. However, the quantum numbers of initial and final states for any physical process coincide.

Let us comment on the definition of quantum numbers in the presence of continuous and finite symmetries, respectively. In both cases, the spectrum of the theory is described using irreducible representations of the symmetry group.

Continuous symmetries

For Lie group representations, the quantum numbers can be obtained as follows.

The so-called Harish-Chandra theorem shows that one can uniquely characterise the irreducible representations of a finite-dimensional semi-simple Lie algebra by their eigenvalues with respect to all the Casimir invariants [115]. Casimir operators are elements of the centre of the enveloping algebra, i.e. they commute with all other elements of the algebra, and they are polynomials of the generators. Each semi-simple Lie algebra $\mathfrak{g}$ has exactly rank $\mathfrak{g}$ independent such operators. The first Casimir operator for $\mathrm{SU}(N)$ groups, for example, can be written [115]

$$C_{\boldsymbol{R}} \coloneqq \delta_{ab}\, \boldsymbol{R}(T^a)\, \boldsymbol{R}(T^b)\,, \tag{13.1}$$

where it is assumed that a basis with a normalised diagonal Killing form is used for the representation $\boldsymbol{R}$ of the generators T^a. Specialising to $\mathrm{SU}(2)$, this operator is just the well-known $\boldsymbol{L}^2$, i.e. the total angular momentum operator. It is already sufficient to distinguish all irreducible representations of $\mathrm{SU}(2)$.

It is also possible to distinguish the different basis vectors within each irreducible module. Some of the required labels are provided by the eigenvalues with respect to the Cartan sub-algebra of the Lie algebra, i.e. the weights. For example, in $\mathrm{SU}(2)$, the Cartan sub-algebra is spanned by $\boldsymbol{L}_z$, whose eigenvalues together with the eigenvalues of the Casimir operator $\boldsymbol{L}^2$ are sufficient to distinguish all states. However, in general, labelling states just using their weights is insufficient. In fact, some of the weights might be degenerate as, for example, the weight $(0, 0)$ of the adjoint representation of $\mathrm{SU}(3)$. Racah [208, 209] showed that one needs $\dim \mathfrak{g}$ operators to distinguish all states, $\operatorname{rank} \mathfrak{g}$ of which are already given by the Casimir operators. Hence, another $\dim \mathfrak{g} - \operatorname{rank}(\mathfrak{g})$ operators must be determined. The $\operatorname{rank} \mathfrak{g}$ elements of the Cartan sub-algebra can be used to supply a subset of these operators, leaving another $(\dim \mathfrak{g} - 3 \operatorname{rank} \mathfrak{g})/2$ operators and their conjugates to be found. Racah also showed that it is always possible to find such a set of operators [208, 210–212].

Finite symmetries

For finite symmetries it is less well known how to construct operators whose eigenvalues can be used as quantum numbers to label states. Let us first fix some notation. The unitary operators $\boldsymbol{U}_g$ implement the group transformation on the field operators, i.e.

$$\boldsymbol{U}_g \, \boldsymbol{\Phi} \, \boldsymbol{U}_g^{-1} = \rho_{\boldsymbol{\Phi}}(g) \, \boldsymbol{\Phi} \,. \tag{13.2}$$

Note that they fulfil the group law

$$\boldsymbol{U}_g \, \boldsymbol{U}_h = \boldsymbol{U}_{hg} \,. \tag{13.3}$$

By assumption, these unitary operators commute with the Hamiltonian.

The operators needed to distinguish the different irreducible representations of a finite group G are the so-called class-operators, cf. e.g. [213]. They are defined as the sum of all operators belonging to group elements in a single conjugacy class,

$$\boldsymbol{K}_m \coloneqq \frac{1}{|C_m|} \sum_{g \in C_m} \boldsymbol{U}_g \,, \tag{13.4}$$

where m is used to label the conjugacy classes C_m of G. The class-operators commute with all other group operators,

$$\begin{aligned} [\boldsymbol{K}_m, \boldsymbol{U}_h] &= \frac{1}{|C_m|} \sum_{g \in C_m} [\boldsymbol{U}_g, \boldsymbol{U}_h] = \frac{1}{|C_m|} \sum_{g \in C_m} (\boldsymbol{U}_h \, \boldsymbol{U}_g \, \boldsymbol{U}_{h^{-1}} \, \boldsymbol{U}_h - \boldsymbol{U}_h \, \boldsymbol{U}_g) \\ &= \frac{1}{|C_m|} \sum_{g \in C_m} (\boldsymbol{U}_h \, \boldsymbol{U}_g - \boldsymbol{U}_h \, \boldsymbol{U}_g) = 0 \,, \end{aligned} \tag{13.5}$$

and, henceforth, all $\boldsymbol{K}_m$ commute amongst each other. Moreover, since all group operators commute with the Hamiltonian, the same is true for the $\boldsymbol{K}_m$ such that they are conserved quantities. As the $\boldsymbol{K}_m$ commute with all group elements, Schur's lemma implies that the class-operators act as multiples of the identity on irreducible representations of the group. Taking the trace one can fix the coefficient and arrives at

$$\boldsymbol{K}_m = \frac{\chi_{\boldsymbol{R}_i}(C_m)}{\dim \boldsymbol{R}_i} \, \mathrm{id} \tag{13.6}$$

for the irreducible representation $\boldsymbol{R}_i$, i.e. the eigenvalues are the characters normalised by the dimension of the irreducible representation.[36]

To be more explicit, let $\boldsymbol{a}_m^\dagger$ be the creation operator in the m-th component of a field operator $\boldsymbol{\Phi}$ which transforms in the irreducible representation $\boldsymbol{R}_i$ of G. Then, assuming an unbroken symmetry, one can compute the action of the n-th class-operator $\boldsymbol{K}_n$ of G on the state created by $\boldsymbol{a}_m^\dagger$ out of the vacuum,

$$\begin{aligned} \boldsymbol{K}_n \, \boldsymbol{a}_m^\dagger |0\rangle &= \frac{1}{|C_n|} \sum_{g \in C_n} \boldsymbol{U}_g \, \boldsymbol{a}_m^\dagger |0\rangle = \frac{1}{|C_n|} \sum_{g \in C_n} \rho_{\boldsymbol{R}_i}(g)_{mk} \, \boldsymbol{a}_k^\dagger |0\rangle =: (K_n)_{mk} \, \boldsymbol{a}_k^\dagger |0\rangle \\ &= \frac{\chi_{\boldsymbol{R}_i}(C_n)}{\dim \boldsymbol{R}_i} \, \boldsymbol{a}_m^\dagger |0\rangle \,, \end{aligned} \tag{13.7}$$

where the matrix K_n was defined. The second line follows from equation (13.6).

Given the class-operators it is possible to define conserved observables [213]

$$\boldsymbol{L}_m = \boldsymbol{K}_m + \boldsymbol{K}_m^\dagger = \boldsymbol{K}_m + \boldsymbol{K}_{m^{-1}} \,, \tag{13.8a}$$

$$\boldsymbol{L}'_m = \mathrm{i}(\boldsymbol{K}_m - \boldsymbol{K}_m^\dagger) = \mathrm{i}(\boldsymbol{K}_m - \boldsymbol{K}_{m^{-1}}) \tag{13.8b}$$

from the $\boldsymbol{K}_m$ that can be used to distinguish states in different irreducible representations. Here $\boldsymbol{K}_{m^{-1}}$ denotes the class-operator of the conjugacy class containing the inverses of the elements of conjugacy class C_m.

The operators thus obtained are the analogues of the Casimir operators of Lie groups. They are sufficient to distinguish between inequivalent irreducible representations but not between states within one irreducible representation space.

One can also label the individual states of an irreducible module. For this one must choose a subgroup H such that the restriction of each irreducible G representation to this subgroup is multiplicity free, i.e. no irreducible representation of H is contained more than once in the decomposition of each irreducible representation of G. Group–subgroup pairs (G, H) where the restriction of each irreducible representation of G to H is multiplicity free are called strong Gelfand pairs. If it is possible to find such a subgroup, one can again compute the class-operators, this time with respect to the subgroup, and use their corresponding observables to distinguish different states in the irreducible module of G [213]. These labels are henceforth called internal quantum numbers of a representation. If a whole chain of such subgroups exists, one can distinguish all the states in an irreducible G module by the constructed observables. If such a chain does not exist, one has to find the additional labelling operators using different means [213].[37]

Example

As an example, take the group $\Delta(27)$, whose details are given in Section A.1.3. As shown in (13.7), the class-operators $\boldsymbol{K}_m$ have as eigenvectors the states $\boldsymbol{a}_m^\dagger |0\rangle$ with eigenvalues proportional to the characters of the representation that the $\boldsymbol{a}_m^\dagger$ reside in. Since the characters separate the irreducible representations, i.e. there is always at least one character that distinguishes between two representations, the $\boldsymbol{K}_m$ are enough to distinguish between states in different irreducible representations of $\Delta(27)$.

36 The quantities $\chi_{\boldsymbol{R}_i}(C_m)$ are well defined since any choice of $g \in C_m$ gives the same value for the character.

37 In a scan with `GAP` up to order 380 (without order 256) we did not find any group without a subgroup that fulfils the criterion. However, Wigner [214] claims that it is not always possible to find such a subgroup.

If one wants to distinguish the different states within the triplet representation of $\Delta(27)$, one can use the class-operators of the $\mathbb{Z}_3$ subgroup generated by the element b. The $\mathbf{3}$ of $\Delta(27)$ decomposes into a $\mathbf{1} \oplus \mathbf{1}' \oplus \mathbf{1}''$ of $\mathbb{Z}_3$, i.e. the decomposition is multiplicity free and $(\Delta(27), \mathbb{Z}_3)$ is a strong Gelfand pair.[38] With respect to this $\mathbb{Z}_3$ subgroup, there are two new non-trivial class-operators $\boldsymbol{K}'_m$, which belong to the two non-trivial conjugacy classes of $\mathbb{Z}_3$. Since $\mathbb{Z}_3$ is abelian, the two conjugacy classes each contain only one element: $C'_1 = \{b\}$ and $C'_2 = \{b^2\}$, i.e. $C'_n = \{b^n\}$. Hence,

$$\boldsymbol{K}'_n \, \boldsymbol{a}^\dagger_m \, |0\rangle = \frac{1}{|C'_n|} \sum_{g \in C'_n} \boldsymbol{U}_g \, \boldsymbol{a}^\dagger_m \, |0\rangle = \frac{1}{1} \sum_{g = b^n} (\rho_{\mathbf{3}}(g))_{mk} \, \boldsymbol{a}^\dagger_k \, |0\rangle = (B^n)_{mk} \, \boldsymbol{a}^\dagger_k \, |0\rangle \ . \tag{13.9}$$

Specialising to the class-operator $\boldsymbol{K}'_1$ – the second one does not offer any additional information – one can verify explicitly the statements made above. It acts as a multiple of the identity on each of the three subspaces $\mathbf{1}$, $\mathbf{1}'$ and $\mathbf{1}''$, namely as 1, ω and ω^2, respectively. Therefore, it provides enough labels to distinguish the three sub-states of the triplet of $\Delta(27)$. Moreover, one can see explicitly that it commutes with all $\boldsymbol{K}_m$ of $\Delta(27)$ because the latter are multiples of the identity on the whole triplet space.

This shows that for a complete labelling of states in the presence of a $\Delta(27)$ symmetry, it suffices to use (a certain subset of) the class-operators $\boldsymbol{K}_m$ of $\Delta(27)$ and the class-operator $\boldsymbol{K}'_1$ of the $\mathbb{Z}_3$ subgroup of $\Delta(27)$. All of these operators commute with each other and, since they are made up of symmetry group elements, with the Hamilton operator.

VII.13.2 Inversion of quantum numbers

After defining the necessary operators, one can discuss the action of CP on the quantum numbers, or rather, define CP as a transformation that acts in a specific way on them.

Continuous symmetries

As already explained, Grimus and Rebelo [14] defined CP via an automorphism that sends each weight to minus itself. Note that these weights constitute the weights of the complex conjugate of the original irreducible representation. This automorphism is uniquely defined by this requirement, up to the choice of Cartan sub-algebra, and is the so-called contragredient automorphism or Chevally involution [14, 115]. Depending on the specific group, it can be a non-inner, as e.g. for $\mathrm{SU}(N)$ with $N > 2$, or an inner, as e.g. for $\mathrm{SO}(2N+1)$ with $N > 1$, automorphism [14].[39] Since the definition of the contragredient automorphism refers to a specific Cartan sub-algebra, the definition of CP might seem to depend on this choice. However, all Cartan sub-algebras and, therefore also their contragredient automorphisms, are connected via inner automorphisms. Thus, the CP transformation defined this way is physically unique.

One has to be careful, however, when saying that all quantum numbers are inverted. The weights of a CP transformed state are minus the weights of the original state; however, not

38 One only has to consider the triplet because all other representations of $\Delta(27)$ are one-dimensional and the $\Delta(27)$ characters are already sufficient to distinguish them.

39 Note that for $\mathrm{SU}(N)$ it is often said that the automorphism related to CP is the diagram automorphism, which sends a weight $\Lambda = (\Lambda^1, \Lambda^2, \dots, \Lambda^{N-1})$ to $(\Lambda^{N-1}, \Lambda^{N-2}, \dots, \Lambda^1)$. This is a representative of the equivalence class of non-inner automorphisms of the outer automorphism group of $\mathrm{SU}(N)$. However, physically one should rather think of a different representative of this class which sends Λ to $(-\Lambda^1, -\Lambda^2, \dots, -\Lambda^{N-1})$ as the defining automorphism of CP. The two automorphisms are related by an inner automorphism and thus give physically identical results [14].

all other quantum numbers are minus their original values. Take, for example, the second order Casimir index defined in (13.1). Sending each weight of a state to minus itself has the same effect on its eigenvalues with respect to C_R as sending T^a to $-(T^a)^T$ in C_R and applying it to the original state. Hence, since the quadratic Casimir is quadratic in the generators, the CP transformed state has the same quantum number as the original state. The same is true for any even-order Casimir operator, while any quantum number with respect to an odd-order Casimir is negated. Instead of insisting on all quantum numbers being negated, one should rather adopt the contragredient automorphism as the defining criterion for a CP transformation as was factually done by Grimus and Rebelo [14]. The result is then completely consistent with the cases of QED and the SM and the criteria outlined in Section VII.4.

Finite symmetries

One can now try to transfer this knowledge to finite groups, where one uses the class-operators of a subgroup chain to label states.

To obtain the commutation relation of the class-operators $\boldsymbol{K}_m$ with the CP operator, one can consider the action of a group element on a CP transformed field operator,[40]

$$\begin{aligned} \boldsymbol{U}_g\,(\boldsymbol{CP})\,\boldsymbol{\Phi}\,(\boldsymbol{CP})^{-1}\,\boldsymbol{U}_g^{-1} &= U_{CP}\,\rho(g)^*\,\boldsymbol{\Phi}^\dagger \\ &= \rho(u(g))\,U_{CP}\,\boldsymbol{\Phi}^\dagger = (\boldsymbol{CP})\,\boldsymbol{U}_{u(g)}\,\boldsymbol{\Phi}\,\boldsymbol{U}_{u(g)}^{-1}\,(\boldsymbol{CP})^{-1}\,. \end{aligned} \tag{13.10}$$

Since the creation operators in $\boldsymbol{\Phi}$ generate a basis for the Hilbert space, it follows that

$$\boldsymbol{U}_g\,(\boldsymbol{CP}) = (\boldsymbol{CP})\,\boldsymbol{U}_{u(g)} \tag{13.11}$$

and, hence, that

$$\boldsymbol{K}_m\,(\boldsymbol{CP}) = (\boldsymbol{CP})\,\boldsymbol{K}_{u(m)}\,. \tag{13.12}$$

Similar to the continuous case, it is inconsistent to define CP by demanding that all quantum numbers be sent to their negative values by CP. However, taking the physical criterion obtained in Section VII.4.2 that the automorphism be class-inverting, one sees that the eigenvalues of a state with respect to the hermitian observables $\boldsymbol{L}_m$ are invariant and the ones with respect to $\boldsymbol{L}'_m$ are inverted. In fact, this holds if and only if the automorphism is class-inverting. Analogous to the continuous case, if a state in the irreducible representation $\boldsymbol{R}$ is CP transformed, its quantum numbers are replaced by the eigenvalues which a state in the complex conjugate representation $\overline{\boldsymbol{R}}$ has. Given the observations made in Section VII.4 and this fact, demanding that the automorphism defining CP be class-inverting seems the correct starting point.

However, in contrast to the continuous case, the effect of the CP transformation on the internal quantum numbers of a representation, i.e. the labels of states within one irreducible representation, is not fixed. Let us thus try to remedy this. The observables needed to distinguish the internal states are the class-operators of some subgroup $H \subset G$. As the discussion in Section VII.12 showed, the restriction of an automorphism to a subgroup is not always an automorphism of the subgroup. Moreover, even if the restriction is an automorphism, it does not have to be class-inverting with respect to the subgroup. An

40 Note that the dagger in $\boldsymbol{\Phi}^\dagger$ denotes the operator adjoint; $\boldsymbol{\Phi}^\dagger$ is still a column vector in the discrete symmetry space.

example of this case is the Bickerstaff–Damhus automorphism of $\mathrm{SG}(54,5) = \Delta(27) \rtimes \mathbb{Z}_2$, whose restriction to $\Delta(27)$ is an automorphism but not class-inverting, as already discussed in Section VII.12.[41]

The general situation is as follows. Let H be a subgroup of G such that

$$\chi^H_{\boldsymbol{R}_i} := \chi_{\boldsymbol{R}_i}\big|_H = \sum_n m_n \chi^H_{\boldsymbol{r}_n}\,, \tag{13.13}$$

with all m_n either zero or one for each irreducible representation $\boldsymbol{R}_i$ of G, i.e. G and H are a strong Gelfand pair, and where $\boldsymbol{r}_n$ are the irreducible representations of H. Furthermore, assume that a class-inverting automorphism u restricts to an automorphism of the subgroup $H \subset G$, i.e. $u(H) = H$. Then it follows that

$$\chi^H_{\boldsymbol{R}_i} \circ u = \chi_{\boldsymbol{R}_i}\big|_H \circ u = \sum_n m_n \chi^H_{\boldsymbol{r}_n} \circ u \tag{13.14a}$$

and by the consistency condition (4.2) that

$$\chi^H_{\boldsymbol{R}_i} \circ u = \left(\chi^H_{\boldsymbol{R}_i}\right)^* = \sum_n m_n \left(\chi^H_{\boldsymbol{r}_n}\right)^*\,. \tag{13.14b}$$

However, the two equations together only show that the set of characters $\chi^H_{\boldsymbol{r}_n} \circ u$ with $m_n = 1$ is equal to the set of characters $\left(\chi^H_{\boldsymbol{r}_n}\right)^*$ with $m_n = 1$, which still leaves the possibility of permuting some of the characters instead of conjugating them, i.e. the automorphism does not have to be class-inverting for the subgroup.

This is precisely what happens in the SG(54,5) case with the (real) representation $\mathbf{6}$, which decomposes as $\mathbf{3} \oplus \overline{\mathbf{3}}$ to $\Delta(27)$. Although, at the level of SG(54,5), the Bickerstaff–Damhus automorphism sends $\mathbf{6}$ to $\overline{\mathbf{6}} = \mathbf{6}$, its restriction to $\Delta(27)$ sends $\mathbf{3}$ to $\mathbf{3}$ and $\overline{\mathbf{3}}$ to $\overline{\mathbf{3}}$. Using the $\Delta(27)$ subgroup to define the internal quantum numbers for SG(54,5), the internal numbers of the hexaplet are not all inverted by the Bickerstaff–Damhus automorphism. This can be seen as the reason why indirect spontaneous CP violation as described in Section VII.9.3 and Section VII.12 is possible.

A sufficient condition for a CP transformation to circumvent this issue is the following. Let CP be defined by a class-inverting automorphism u of G such that for some subgroup chain $G = G_0 \supset G_1 \supset \cdots \supset G_n$ with an abelian group G_n the following conditions hold for all $i = 1, \ldots, n$:

$$u(G_m) = G_m \tag{13.15a}$$

and

$$\forall g_m \in G_m \, \exists\, h \in G_{m+1} : u(g_m) = h\, g_m^{-1}\, h^{-1}\,. \tag{13.15b}$$

These two conditions ensure that one can define quantum numbers because the restrictions of representations along the subgroup chain are multiplicity free, see the proof in Section A.5, and, at the same time, that the each restriction of the automorphism is class-inverting.

The automorphism used in the SG(54,5) example does not fulfil the second condition. Using the $\mathbb{Z}_3 \times \mathbb{Z}_3$ subgroup to label the states, there is no class-inverting automorphism of the full group which is also class-inverting when restricted to this subgroup, as can easily be checked with GAP.

41 Note that SG(54,5) and $\Delta(27)$ form a strong Gelfand pair.

There is a second issue associated to the internal quantum numbers which cannot be resolved by attaching more conditions to CP transformations. Whereas the concept of weight for continuous groups is unique up to inner automorphisms of the Lie algebra, this is not the case for the internal quantum numbers of discrete groups. In fact, their definition relied on some choice of subgroup H of G. Even demanding that they should form a strong Gelfand pair, this choice is by far not unique. An automorphism of G whose restriction to H is not class-inverting might be class-inverting when restricted to a different subgroup H'.

As this difficulty cannot easily be resolved and since with indirect spontaneous CP violation it is not possible to generate a non-trivial δ_{CP} in the SM, see Section VII.12, it does not seem worthwhile to try to fix the action of CP on internal quantum numbers for discrete symmetries. One should, however, keep in mind that indirect spontaneous CP violation can happen due to this omission. Thus, the only sensible stringent condition on CP transformations of discrete groups is the one already obtained in Section VII.4: the automorphism should be class-inverting.

VII.14 Conclusion of the chapter

The discussion in this chapter shows clearly that the generalisation of CP to models with discrete non-abelian symmetries is non-trivial. As was demonstrated, in order to obtain a physical CP transformation, the consistency condition of Holthausen, Lindner and Schmidt [15] and Feruglio, Hagedorn and Ziegler [16] relating a CP transformation to an automorphism of the discrete group is insufficient in generic settings. This deficiency was shown to be cured by the additional constraint that the automorphism must be class-inverting. In this case, each field can be sent to its own complex conjugate such that the decisive characteristic of the CP transformations of QED and the SM is retained. For all practical purposes, it is also possible to restrict the discussion to involutory automorphisms.

Since not every group has class-inverting automorphisms, the existence of a consistent CP transformation for generic settings is a non-trivial constraint. Thus, the discrete groups were shown to fall into three separate classes: type I groups with no consistent CP transformation in generic settings, an important example for which are odd-order non-abelian groups, type II A groups, for which in a certain basis the canonical CP transformation can be used, and type II B groups, for which only non-canonical CP transformations are available.

The consistency of the canonical CP transformation, at least in a certain basis, was related to the existence of a basis with real Clebsch–Gordan coefficients using a theorem by Bickerstaff and Damhus [164]. Moreover, a useful tool to check whether an automorphism is class-inverting was provided with the twisted Frobenius–Schur indicator.

As was discussed in detail, the constraints on couplings due to generalised CP transformations depend on the type of the automorphism. For type II A, only the phases of couplings are constrained, in analogy to the continuous group case. In type II B cases, some couplings are completely forbidden by a $\mathbb{Z}_2$ symmetry which is fully determined by the CP transformation. The phases of all other couplings are constrained as for type II A or continuous groups. In type I cases with a non-generic representation content, either the phases of couplings are constrained or several couplings are related in a non-trivial way, e.g. such that their absolute values are identical and their phases conjugate to each other. This peculiar behaviour does not exist for the other types of groups.

The properties of models using a type I symmetry with a sufficiently generic representation content to render the introduction of a CP transformation impossible were discussed using

an example based on $\Delta(27)$. Moreover, it was demonstrated that this toy model can be obtained by spontaneous breaking from a model with a larger type II symmetry group, namely SG(54,5), in such a way that all phases are fixed by the group theory of the model. This type of models offers an interesting avenue for further studies.

Furthermore, the model of geometrical CP violation by Branco, Gerard and Grimus [17], which is also based on $\Delta(27)$, was reviewed and the essence of this effect highlighted. Thereby, the common misunderstanding that non-trivial relative phases in the VEV are sufficient for geometrical CP violation was corrected.

Using the information gained on generalised CP transformations, the strong CP problem of the Standard model was re-considered. Although a precise understanding of CP transformations is, of course, indispensable for its solution, it turned out that generalised CP transformations do not yield any genuinely new insights.

The properties of CP symmetries concerning the spontaneous breaking of discrete symmetries were investigated. Not only can CP be broken spontaneously directly by the VEV, but also indirectly by the breaking of the discrete group. This could already be seen in the modification of the $\Delta(27)$ toy example, where the CP symmetry is broken spontaneously although the VEV itself is CP invariant. In fact, the breaking of the discrete group SG(54,5) to $\Delta(27)$ turns a class-inverting automorphism, which defines a consistent CP transformation, into a non-class-inverting automorphism, which is not sufficient to guarantee CP invariance.

Finally, the definition of CP was further investigated using the concept of quantum numbers for discrete groups in analogy to the discussion of continuous groups started by Grimus and Rebelo [14]. Unfortunately, no further unambiguous constraints could be found. However, the indirect CP violation in the SG(54,5) model could be traced back to the fact that some internal quantum numbers are not inverted in the first place.

In the following section, some claims from the literature concerning generalised CP transformations are critically reviewed.

VII.15 Comments on claims in the literature

At this point, some comments on claims in the literature connected to the generalised CP transformations discussed in this chapter seem appropriate. Indeed, it is shown that some of these claims do not withstand closer scrutiny. The publications to be commented on are the following:

(i) 'Towards realistic models of quark masses with geometrical CP violation' by Medeiros Varzielas and Pidt [215];

(ii) 'Lepton Mixing Predictions including Majorana Phases from $\Delta(6n^2)$ Flavour Symmetry and Generalised CP' by King and Neder [216];

(iii) 'Invariant approach to CP in family symmetry models' by Branco, Medeiros Varzielas and King [217].

The discussions below are not self-contained and can only be understood in comparison with the original publications. Equation numbers mentioned below refer to the journal versions in cases (i) and (ii) and to *arXiv* version v1 for (iii).

VII.15.1 Comments on 'Towards realistic models of quark masses with geometrical CP violation'

Medeiros Varzielas and Pidt [215] claim to have built a semi-realistic model of quark masses with geometrical CP violation. It can be shown, however, that their CP violation is not really geometrical in the sense defined by Branco, Gerard and Grimus [17] and discussed in Section VII.10 because CP is also explicitly violated by the Yukawa matrices.

The three Higgs doublet potential with $\Delta(27)$ symmetry of [17] was discussed in some detail already in Section VII.10.1. Here, only the parts relevant to the present discussion are repeated. Let H be the triplet of Higgs doublets. The potential of [17], see also equation (10.1), leads indeed, as assumed by [215], to the vacuum expectation value

$$\langle H \rangle = v\,(\omega,\, 1,\, 1)^T\,, \tag{15.1}$$

where only the charge zero component of the doublets is displayed. At least, this is true if the CP transformation

$$H \overset{CP}{\longmapsto} H^* \tag{15.2}$$

is used to constrain the phases in the Higgs potential.[42] As can easily be seen, this CP transformation is spontaneously broken by the vacuum expectation value.

Moreover, Medeiros Varzielas and Pidt [215] use as Yukawa Lagrangian for the down-type quarks [215, equations (2)-(4)]

$$\begin{aligned}\mathcal{L}_d = {} & y_3\, Q_3\, (H\, d^c)_{01} + y_2\, Q_2\, (H\, d^c)_{00}\, \varphi^2 + y_1\, Q_1\, (H\, d^c)_{00}\, \varphi^3 + \\ & + p_2\, Q_2\, (H\, d^c)_{01}\, \theta + p_1\, Q_1\, (H\, d^c)_{01}\, \varphi\, \theta + \\ & + h_3\, (H\, H^\dagger)\, Q_3\, (H\, d^c)_{01} + h_2\, (H\, H^\dagger)\, Q_2\, (H\, d^c)_{00}\, \varphi^2 + h_1\, (H\, H^\dagger)\, Q_1\, (H\, d^c)_{00}\, \varphi^3\,.\end{aligned} \tag{15.3}$$

For the notation used see the original paper, its details are not really needed for the following discussion.

It should be clear from (15.3) that the phases of the couplings h_i are exactly the same as the phases of the corresponding couplings y_i no matter which CP transformation is imposed on the model because $(H\,H^\dagger)$ is invariant under any CP transformation. Thus, the partial mass matrices obtained from the first and third line, respectively, called M and M_h in [215], are identical up to a factor of v^2 and the replacement of y_i with h_i, where $y_i = c_i\, h_i$ with $c_i \in \mathbb{R}$. That is, the matrices M and M_h of [215] should have identical structures. However, Medeiros Varzielas and Pidt [215] claim to have obtained

$$M = v \begin{pmatrix} y_1\,\omega & y_1 & y_1 \\ y_2\,\omega & y_2 & y_2 \\ y_3 & y_3 & y_3\,\omega \end{pmatrix}, \tag{15.4}$$

$$M_h = v^3 \begin{pmatrix} h_1 & h_1\,\omega^2 & h_1\,\omega^2 \\ h_2 & h_2\,\omega^2 & h_2\,\omega^2 \\ h_3\,\omega^2 & h_3\,\omega^2 & h_3 \end{pmatrix}. \tag{15.5}$$

42 Unfortunately, Medeiros Varzielas and Pidt [215] do not indicate which kind of CP transformation they use. Since the canonical CP transformation leads to the desired VEV, this seems to have been their choice. In fact, the specific choice does not matter for the following discussion.

In fact, these different structures, as they realise themselves, are the reason for a non-trivial δ_{CP} in the model. That is, Medeiros Varzielas and Pidt [215] choose different phases for the h_i than for the y_i by hand, thereby breaking the CP transformation explicitly, in order to generate a non-trivial δ_{CP}. This should, of course, not be called geometrical CP violation.

Imposing instead the CP transformation (15.2) consistently on the Lagrangian, the couplings y_i, p_i and h_i of the Yukawa terms (15.3) are real. Then, the correct mass matrices are M as shown in (15.4) and a matrix M'_h obtained from this M by multiplication with v^2 and the replacement of the real couplings y_i with some real h_i. However, following this consistent procedure, CP is only violated in the Higgs potential but not in the Yukawas, i.e. $\delta_{CP} = 0$. This is, of course, a tree level statement in the sense that the quantum corrected mass matrices could, in principle, receive corrections from the Higgs self-interactions that lead to a non-zero effective δ_{CP}. It seems unlikely, though, that this induces a realistically large CP violation in the quark sector.

VII.15.2 Comments on 'Lepton Mixing Predictions including Majorana Phases from $\Delta(6n^2)$ Flavour Symmetry and Generalised CP'

King and Neder [216] make several claims about CP transformations for the discrete SU(3) subgroups in the $\Delta(6\,n^2)$ family.

First of all, King and Neder [216] claim that: 'An outer automorphism however is not inner […], i.e. there is at least one $g' \in G$ which is not mapped back into its original conjugacy class' [216]. Further: 'This proves also that an automorphism that maps each element back into its original conjugacy class is inner' [216]. However, the notion of class-preserving automorphisms is distinct from the notion of inner automorphisms. Such a counter-example of a class-preserving non-inner automorphism exists, for example, for the group SG(32,43), as can be easily checked with GAP, see also the list in Appendix D. That is, the statement cited above is wrong.

Moreover, they claim that their operation in [216, equation (19)] 'can be thought of as an automorphism mapping $g \mapsto g^{-1}$ followed by an automorphism that maps g^{-1} onto another element in the same class' [216]. However, the inversion map $g \mapsto g^{-1}$ is not an automorphism but an anti-automorphism as it changes the order of its arguments. Only for abelian groups these two notions coincide. To see this, assume that τ is an automorphism and sends each group element to its inverse. Then

$$gh = \tau(g^{-1})\,\tau(h^{-1}) = \tau\left(g^{-1}h^{-1}\right) = \tau\left((hg)^{-1}\right) = hg\,, \qquad \forall\, g,h \in G\,, \tag{15.6}$$

which proves that the group is abelian. The statement cited above is thus wrong for any non-abelian group and therefore, in particular, for the $\Delta(6\,n^2)$ family.

Furthermore, the assumption that a matrix w_r exists fulfilling the properties assumed by King and Neder in [216, equation (19)] is the same as assuming that there is a class-inverting automorphism. However, there is, for example, no class-inverting automorphism for $\Delta(54)$. Moreover, in [216, equation (21)], the inverse of the representation map is applied to something that by no means has to be the representation matrix of a group element, i.e. the map is acting on something on which it is not even defined. Therefore, any of the statements by King and Neder following [216, equation (19)] are not proved. They could only be true by accident.

As can easily be seen, even this is not the case for their final group theoretical statement, where X_r is what is called U_{CP} in our notation and the representation considered is assumed

to be faithful:[43]

> In [15] the authors show that only gCP transformations that map elements into the class of its inverse element make observables conserve CP. We have proved here that such transformations are given by $X_r \in e^{i\alpha} G$. In the following we will specialise G to be $\Delta(6n^2)$. [216]

First of all, it is clear from the discussion in Section VII.3.2 that the CP transformation that they claim gives the correct result would be physically equivalent to the canonical CP transformation. The group element is just a symmetry transformation and can be dropped and the phase can be absorbed in a re-phasing of the field operators. Their statement is thus equivalent to saying that a consistent CP transformation for the $\Delta(6n^2)$ family is the canonical CP transformation.[44] This statement is clearly basis-dependent.[45] Even ignoring this issue, the canonical CP transformation is not consistent with every $\Delta(6n^2)$ symmetry. In fact, as already mentioned, $\Delta(54)$ is of type I, i.e. it has no class-inverting automorphism at all. This can easily be checked with the GAP codes provided in Appendix C. Thus, neither the canonical CP transformation nor any other CP transformation can be consistent with the $\Delta(54)$ symmetry.

VII.15.3 Comments on 'Invariant approach to CP in family symmetry models'

Branco, Medeiros Varzielas and King [217] discuss the invariant approach to CP violation and its relation to the consistency condition used in the present work.[46] They claim the following, where their citation [11] refers to the consistency condition by [15, 16]:

> We show that such an approach, which relies on a knowledge of the Lagrangian of the model, is complementary to the approach based on the consistency relations [11]. Indeed we will show how the consistency conditions can be derived from the requirement that the Lagrangian is invariant under both CP symmetry and the discrete family symmetry. Therefore, in analysing particular models, the use of weak basis invariants alone is both sufficient and convenient. [217]

And further:

> The first point we wish to make is that, once a Lagrangian is specified, which is invariant under a family symmetry G and some CP transformation, then the consistency relations [11] are automatically satisfied. [217]

This is certainly not true. As seen already in the example in Section VII.3.2, implementing an inconsistent CP transformation forbids many additional terms. Of course, the CP transformation and the final symmetry group G' obtained by implementing both G and CP are, in a sense, consistent by construction. However, G' is much larger than the desired symmetry G in this case. In fact, one usually ends up with a free theory if G and CP are inconsistent such that G' is at least some continuous unitary group. G' is only the same as G for a CP transformation that fulfils the condition (4.24). This was precisely the constraint

43 Note that their citation [15] is [3].

44 In fact, as can be seen from the last sentence of the quote, they claim to have proved that for all groups G and specialise to $\Delta(6n^2)$ only later.

45 A basis transformation acts differently on the group elements than on U_{CP}, see (3.6). Note, moreover, that they do not refer to any specific basis in their derivation.

46 See also their extended version [218].

used by Holthausen, Lindner and Schmidt [15] and reviewed in Section VII.3.2. The use of weak basis invariants alone is thus not sufficient in the sense claimed by Branco, Varzielas and King [218].

Let us point out why their attempt to prove their statements is insufficient. They consider some mass matrix m and define $H := m\,m^\dagger$. This matrix is assumed to be invariant under group transformations, i.e. [217, equation (6)]

$$\rho(g)^\dagger\, H\, \rho(g) = H\,. \tag{15.7}$$

Moreover, H is assumed to be CP invariant [217, equation (7)],

$$U^\dagger\, H\, U = H^*\,, \tag{15.8}$$

where U is what would here be called U_{CP}. After inserting these two assumptions several times into each other, they end up with [217, equation (10)]

$$U\,(\rho(g)^\dagger)^*\, U^\dagger\, H\, U\, \rho(g)^*\, U^\dagger = H = \rho(g')^\dagger\, H\, \rho(g') \tag{15.9}$$

which is supposed to hold 'for a g' ' [217]. This equation is, due to the assumptions, correct. However, they claim that comparing its two sides one obtains [217, equation (11)]

$$U\,\rho(g)^*\, U^\dagger = \rho(g')\,. \tag{15.10}$$

This, they claim further, 'is just the consistency relation [11]' [217]. This is incorrect. By the same logic,

$$U\,\rho(g)^*\, U^\dagger = \mathbb{1} \tag{15.11}$$

would have to be true (compare the left-hand side of (15.9) with the middle of the same equation). And, indeed, for fixed g,

$$U\,\rho(g)^*\, U^\dagger = \rho(g') \tag{15.12}$$

would be true for any $g' \in G$, not just for a single one. This is clearly inconsistent.

The reason for this inconsistency and for the breakdown of the proof is the wrong conjecture that one could obtain the implication $A = B$ from a matrix equation

$$A\,H\,A^{-1} = B\,H\,B^{-1} \tag{15.13}$$

independently of what H is. Indeed, the assumptions (15.7) and (15.8) on H are precisely such that equation (15.9) is meaningless in the following sense. Applying (15.7) and (15.8) repeatedly, one immediately sees that equation (15.9) merely is the equality

$$H = H = H\,, \tag{15.14}$$

written in a much more complicated way. That is, equation (15.9) is, under the given assumptions, trivial. Of course, it is impossible to deduce the consistency condition from this relation. Thus, the invariant approach and the consistency condition are not proved to be equivalent.

VIII Conclusion and outlook

The flavour puzzle is one of the most important unsolved problems of particle physics. For a complete understanding of Nature, it seems indispensable to derive the observed patterns of masses and mixing angles as well as the presence and size of CP violation from some fundamental principle. One framework that could provide such insights is given by discrete non-abelian flavour symmetries. This thesis derived some of the essential ingredients to build meaningful and predictive models within this framework.

For model building with discrete groups, a sound knowledge of finite group theory is necessary. Therefore, a brief introduction to this topic was given in Chapter II. Most importantly, the notion of Clebsch–Gordan coefficients was reviewed, which are needed to construct group invariant Lagrangians. Several ambiguities concerning the definition of these Clebsch–Gordan coefficients that have led to some confusion among model builders were clarified.

As the main reason for the use of discrete symmetries in model building is the quest for a solution to the flavour problem, the flavour sector of the Standard Model was reviewed in Chapter III, and the notion of CKM and PMNS matrices was carefully defined. Several virtues of discrete non-abelian symmetries were detailed, such as that they can predict a non-trivial mixing structure due to their higher-dimensional representations. Further, it was highlighted that the choice of discrete symmetries is supported by the fact that no massless Goldstone bosons emerge when spontaneously breaking the symmetry. Moreover, these symmetries can be obtained both from string theory and by breaking a non-abelian continuous gauge group at very high energies such that they are shielded from possible violations by gravitational effects. As an example of such flavour theories, a model originally presented by Altarelli and Feruglio [9, 10], which is based on the tetrahedral symmetry group A_4, was reviewed. This model predicts at leading order tri-bi-maximal mixing for the neutrinos.

As is well known, symmetries of a classical theory are not always symmetries of the corresponding quantum theory. The failure of this equivalence of classical and quantum symmetries is called anomaly. Not only continuous symmetries are plagued by anomalies, but also discrete symmetries, as can in both cases be seen directly from the symmetry transformation properties of the path integral measure. In Chapter IV, conditions were derived for discrete symmetries to be anomaly free based on the observation that the path integral measure transforms in a proper one-dimensional representation of the group. Indeed, it turned out that this allows for a simple proof of the fact that perfect, and therefore also simple, non-abelian discrete groups are always anomaly free. Moreover, it could be shown that discrete groups in models with $SO(N)$ or exceptional gauge groups are less in danger of anomalies than in models with $SU(N)$ or $Sp(2N)$ gauge groups. Furthermore,

general conditions were derived that connect anomaly freedom of a discrete group to the size of its Abelianisation. A further investigation into the specific effects of anomalously broken discrete symmetries seems worthwhile. In particular, it would be interesting to examine whether one can quantify the effects similarly to the case of anomalous Ward identities for continuous symmetries.

Subsequently, in Chapter V, corrections to neutrino mixing due to additional interactions connecting flavons and the lepton kinetic terms in models with discrete non-abelian symmetries were discussed. Such interaction terms are present in any effective field theory model with discrete non-abelian symmetries. In the supersymmetric case, they are part of the Kähler potential, in which case the corrections are also called Kähler corrections. In both a supersymmetric and a non-supersymmetric example, these kinetic term corrections were shown to be non-negligible. Indeed, under certain circumstances they are large and then drastically change the predictions obtained assuming canonical kinetic terms. This can be used to render otherwise ruled-out models realistic again as shown for the A_4 example. Unfortunately, at the same time, the missing knowledge about the higher-order corrections to the kinetic terms in effective field theories introduces a large ambiguity into the derivation of model predictions. It seems thus important to study UV completions of such flavour models to obtain more information on the size of the effects to be expected. In the supersymmetric case, future limits on flavour changing neutral currents could also be used indirectly to constrain the Kähler potential. In the meantime, making assumptions on the coupling sizes, estimates of the corrections to neutrino mixing can easily be obtained using the analytical formulas derived here and the associated MATHEMATICA package `KaehlerCorrections`.[1]

As mentioned before, due to the conjectured violation of global symmetries by gravitational effects, it seems desirable to obtain discrete symmetries either from string theory or by spontaneous breaking of a continuous gauge group. The latter possibility requires knowledge of the branching rules of representations of the Lie group into representations of the finite subgroup. For example, only vacuum expectation values of fields in non-trivial representations of the Lie group which contain at least one trivial singlet of the subgroup are candidates for the breaking. A procedure for the computation of these branching rules for the case of the compact classical Lie groups and their finite subgroups was presented in Chapter VI. The resulting routines were also implemented in the MATHEMATICA package `DecomposeLGReps` for $U(N)$, $SU(N)$, $SO(N)$ and $USp(2N)$.[2] The method made use of the Weyl character formula for the computation of Lie algebra characters and of their connection to Lie group characters. A finite subgroup was embedded into the Lie group by stating an explicit matrix representation of the finite group that was then interpreted as the restriction of the fundamental representation of the Lie group to the subgroup. Using the Weyl character formula, it was thus shown how to compute in this scenario the characters of arbitrary Lie group representations for all group elements which are also contained in the finite subgroup. The desired branching rules were then determined from the usual scalar product of characters. Using this technique, explicit rules were compiled for some finite groups popular in model building, e.g. A_4, S_4 and $\Delta(27)$, thereby showing that the representation content obtained by such a breaking cannot, in general, be considered generic. It seems thus again important to work with UV completions rather than effective theories or, at least, to take into account such restrictions during the construction of effective models.

The discussion of CP transformations in the presence of discrete non-abelian symmetries presented in Chapter VII turned out to be more complicated but also richer than the

1 http://einrichtungen.ph.tum.de/T30e/codes/KaehlerCorrections
2 http://einrichtungen.ph.tum.de/T30e/codes/DecomposeLGReps

analogous discussion for continuous symmetries. First, the CP transformations of QED and of the Standard Model were introduced. Then the claims on the generalisation of CP to models with additional continuous and discrete symmetries by Grimus and Rebelo [14], Holthausen, Lindner and Schmidt [15] and Feruglio, Hagedorn and Ziegler [16] were reviewed. It was shown that in the discrete group case, contrary to earlier statements, a physical CP transformation cannot be obtained from an arbitrary automorphism of the group. Instead, only class-inverting automorphisms can be used to obtain physical CP transformations. Further, it was argued that in all practical cases the discussion of CP can be restricted to involutory automorphisms. The consistency of the canonical CP transformation was then connected using a theorem by Bickerstaff and Damhus [164] to the existence of a certain kind of class-inverting automorphism and the reality of all Clebsch–Gordan coefficients of the group.

After introducing the twisted Frobenius–Schur indicator as a useful mathematical tool, these newly obtained criteria were used to categorise finite groups into three classes. For type II groups, it is always possible to define CP transformations, regardless of the field content. Indeed, for type II A groups, it is even possible to work with the canonical CP transformation, at least in certain bases. For type II B groups, however, this is impossible, although one can still always consistently define CP. In addition, a type II B group gets possibly enlarged by a commuting $\mathbb{Z}_2$ factor when imposing CP invariance. In contrast to type II groups, type I groups do not allow CP to be consistently defined in generic settings. Only for certain choices of field content could this be achieved. Explicit example groups were discussed for each of the three types. For example, the well-known group $\Delta(27)$ is type I, i.e. it does not allow for a consistent CP transformation in a generic setting. Further, embedding $\Delta(27)$ into a type II A group, a toy model with spontaneous CP violation with group theoretical phases was presented. In fact, CP in this model was broken spontaneously but indirectly by breaking the type II to a type I discrete group. Building a realistic model with such an indirect breaking seems an invigorating possibility for future research.

Further, the effect called geometrical CP violation appearing in the three Higgs doublet model by Branco, Gerard and Grimus [17] was reviewed and some misunderstandings concerning this effect corrected. Indeed, geometrical CP violation is not signalled by just some relative phases of components of a single VEV but by an interplay of phases in the CP transformation matrix and the VEV and the fact that these phases do not continuously depend on couplings. In addition, the newly gained insights on CP transformations were applied to the strong CP problem, where, however, no genuinely new approach to a solution could be found. Furthermore, the spontaneous symmetry breaking of discrete groups in the presence of CP symmetries was studied. Finally, the definition of CP was re-considered regarding the requirement of the inversion of quantum numbers that was first mentioned by Grimus and Rebelo [14]. It turned out that this criterion cannot be imposed in an unambiguous manner and does hence not lead to any additional requirements for CP transformations in the discrete group case.

The results derived here show that particular care must be exercised when building models with discrete non-abelian symmetries. Many subtleties emerge from the group theory of discrete symmetries that are irrelevant in the continuous case. Given the many virtues of discrete symmetries for model building, it seems nonetheless worthwhile to continue with the construction of models incorporating such symmetries. Especially type I groups are appealing candidates for further investigations due to their CP violating properties. Building a realistic example of a full flavour model based on a type I group might be a first step towards a group theoretical explanation of CP violation in the Standard Model.

A Mathematical appendix

In this appendix, the notations and basis conventions for the groups used in the examples of the main text are fixed, and the corresponding Clebsch–Gordan coefficients are shown. Moreover, some more mathematical results are presented that were omitted in the main text.

A.1 Selected finite groups

In the following, some details on the finite groups used most extensively in the main text are provided. Groups are defined by their presentation, i.e. a set of (abstract) generators and their relations.

Moreover, character tables for the groups are shown, i.e. tables with one row for each inequivalent irreducible representation and one column for each conjugacy class with the corresponding characters at the intersections. The conjugacy classes are labelled by the order of their elements and a letter. The second line of a character table shows the cardinality and the third line a representative of each conjugacy class.

Furthermore, explicit matrix realisations for the irreducible representations are displayed together with the corresponding Clebsch–Gordan coefficients. Note that one-dimensional representation matrices can be read off directly from the character table and are thus not shown again. For convenience, the normalisation of the Clebsch–Gordan coefficients is chosen such that the Clebsch–Gordan matrices are unitary.

For other collections of group bases and Clebsch–Gordan coefficients, cf. [15, 57, 58, 73]. Many of the results displayed here were obtained with the help of GAP [20] and the MATHEMATICA package `Discrete` [158].

A.1.1 The tetrahedral group A_4

The tetrahedral group is the symmetry group of the regular tetrahedron. It is isomorphic to the alternating group on four letters A_4 and is generated by two elements s and t with

$$s^2 = t^3 = (st)^3 = e\,. \tag{1.1}$$

The character table of A_4 is shown as Table A.1.

A_4 has four inequivalent irreducible representations: three singlets $\mathbf{1}$, $\mathbf{1}'$ and $\mathbf{1}''$ and one

	C_{1a}	C_{3a}	C_{2a}	C_{3b}
	1	4	3	4
A_4	e	t	s	t^2
1	1	1	1	1
1′	1	ω	1	ω^2
1″	1	ω^2	1	ω
3	3	0	−1	0

Table A.1: Character table of A_4, where $\omega := e^{2\pi i/3}$.

triplet **3**. The choice of basis in this text for the triplet is

$$S := \rho_{\mathbf{3}}(s) = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}, \tag{1.2a}$$

$$T := \rho_{\mathbf{3}}(t) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \tag{1.2b}$$

where $\omega := e^{2\pi i/3}$. This basis is actually a CP basis, i.e. all Clebsch–Gordan coefficients are real.

The only non-trivial tensor product is

$$\mathbf{3} \otimes \mathbf{3} \cong \mathbf{1} \oplus \mathbf{1}' \oplus \mathbf{1}'' \oplus \mathbf{3}_s \oplus \mathbf{3}_a\,, \tag{1.3}$$

where $\mathbf{3}_s$ and $\mathbf{3}_a$ denote the symmetric and the anti-symmetric triplet combinations, respectively. Other linear combinations would, of course, also be possible. In terms of the components of two triplets $\boldsymbol{a}$ and $\boldsymbol{b}$,

$$(\boldsymbol{a} \otimes \boldsymbol{b})_{\mathbf{1}} = \frac{1}{\sqrt{3}}\,(a_1 b_1 + a_2 b_3 + a_3 b_2)\,, \tag{1.4a}$$

$$(\boldsymbol{a} \otimes \boldsymbol{b})_{\mathbf{1}'} = \frac{1}{\sqrt{3}}\,(a_3 b_3 + a_1 b_2 + a_2 b_1)\,, \tag{1.4b}$$

$$(\boldsymbol{a} \otimes \boldsymbol{b})_{\mathbf{1}''} = \frac{1}{\sqrt{3}}\,(a_2 b_2 + a_1 b_3 + a_3 b_1)\,, \tag{1.4c}$$

$$(\boldsymbol{a} \otimes \boldsymbol{b})_{\mathbf{3}_s} = \frac{1}{\sqrt{6}}\begin{pmatrix} 2a_1 b_1 - a_2 b_3 - a_3 b_2 \\ 2a_3 b_3 - a_1 b_2 - a_2 b_1 \\ 2a_2 b_2 - a_1 b_3 - a_3 b_1 \end{pmatrix}, \tag{1.4d}$$

$$(\boldsymbol{a} \otimes \boldsymbol{b})_{\mathbf{3}_a} = \frac{1}{\sqrt{2}}\begin{pmatrix} a_2 b_3 - a_3 b_2 \\ a_1 b_2 - a_2 b_1 \\ a_3 b_1 - a_1 b_3 \end{pmatrix}. \tag{1.4e}$$

Note that the triplet is a real representation. One can hence change to a realisation in which all representation matrices are manifestly real. The relation between the original basis and this new basis denoted with tildes is given by $\tilde{S} := U_\omega\, S\, U_\omega^\dagger$ and $\tilde{T} := U_\omega\, T\, U_\omega^\dagger$ with

$$U_\omega := \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}. \tag{1.5}$$

	C_{1a}	C_{3a}	C_{4a}	C_{2a}	C_{3b}	C_{6a}	C_{6b}
	1	4	6	1	4	4	4
T′	e	t	s	s^2	t^2	$s^2\,t$	$s^2\,t^2$
$\mathbf{1}_0$	1	1	1	1	1	1	1
$\mathbf{1}_1$	1	ω	1	1	ω^2	ω	ω^2
$\mathbf{1}_2$	1	ω^2	1	1	ω	ω^2	ω
$\mathbf{2}_0$	2	-1	0	-2	-1	1	1
$\mathbf{2}_1$	2	$-\omega$	0	-2	$-\omega^2$	ω	ω^2
$\mathbf{2}_2$	2	$-\omega^2$	0	-2	$-\omega$	ω^2	ω
$\mathbf{3}$	3	0	-1	3	0	0	0

Table A.2: Character table of T′, where $\omega := \mathrm{e}^{2\pi\,\mathrm{i}\,/3}$.

The result for the generators in the triplet representation is

$$\tilde{S} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{1.6a}$$

$$\tilde{T} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \tag{1.6b}$$

Note that the VEV $(v, v, v)^T$ in one basis is mapped to the VEV $\sqrt{3}\,(v, 0, 0)^T$ in the other basis, and vice versa.

A.1.2 The double tetrahedral group T′

The double covering of the tetrahedral group is denoted by T′. It is generated by two elements s and t with

$$s^4 = t^3 = (st)^3 = e\,. \tag{1.7}$$

There are seven irreducible representations, $\mathbf{1}_i$, $\mathbf{2}_i$ and $\mathbf{3}$, where $i = 0, 1, 2$. The representations $\mathbf{1}_1$ and $\mathbf{2}_1$ are conjugate to $\mathbf{1}_2$ and $\mathbf{2}_2$, respectively, $\mathbf{2}_0$ is pseudo-real, and $\mathbf{1}_0$ and $\mathbf{3}$ are real. The characters of T′ are shown in Table A.2.

The non-trivial T′ tensor product rules are

$$\mathbf{2}_i \otimes \mathbf{2}_j \cong \mathbf{3} \oplus \mathbf{1}_{i+j \pmod 3}\,, \tag{1.8a}$$

$$\mathbf{2}_i \otimes \mathbf{3} \cong \mathbf{2}_0 \oplus \mathbf{2}_1 \oplus \mathbf{2}_2\,, \tag{1.8b}$$

$$\mathbf{3} \otimes \mathbf{3} \cong \mathbf{1}_0 \oplus \mathbf{1}_1 \oplus \mathbf{1}_2 \oplus \mathbf{3}_\mathrm{s} \oplus \mathbf{3}_\mathrm{a}\,. \tag{1.8c}$$

Ma–Rajasekaran basis

The A_4 basis by Ma and Rajasekaran [192] has a manifestly real triplet representation. It can be complemented to a basis for T′.

$$\rho^{\mathrm{M}}_{\mathbf{2}_i}(s) = -\frac{1}{\sqrt{3}} \begin{pmatrix} \mathrm{i} & \sqrt{2}\,\mathrm{i} \\ \sqrt{2}\,\mathrm{i} & -\mathrm{i} \end{pmatrix}, \qquad i = 0, 1, 2\,, \tag{1.9a}$$

$$\rho^{\mathrm{M}}_{\mathbf{2}_0}(t) = \begin{pmatrix} \omega^2 & 0 \\ 0 & \omega \end{pmatrix}, \qquad \rho^{\mathrm{M}}_{\mathbf{2}_1}(t) = \begin{pmatrix} 1 & 0 \\ 0 & \omega^2 \end{pmatrix}, \qquad \rho^{\mathrm{M}}_{\mathbf{2}_2}(t) = \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix}, \tag{1.9b}$$

$$\rho^{\mathrm{M}}_{\mathbf{3}}(s) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad \rho^{\mathrm{M}}_{\mathbf{3}}(t) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}. \tag{1.9c}$$

The component expressions of the tensor products in this basis are shown below with normalisation such that the Clebsch–Gordan matrices are unitary. The overall phases are obtained via a basis transformation from the CP basis, see below.

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{1}_0} = \frac{x_1 y_1 + x_2 y_2 + x_3 y_3}{\sqrt{3}}, \tag{1.10a}$$

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{1}_1} = \frac{x_1 y_1 + \omega^2 x_2 y_2 + \omega x_3 y_3}{\sqrt{3}}, \tag{1.10b}$$

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{1}_2} = \frac{x_1 y_1 + \omega x_2 y_2 + \omega^2 x_3 y_3}{\sqrt{3}}, \tag{1.10c}$$

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{3}_\mathrm{s}} = \frac{1}{\sqrt{2}} \begin{pmatrix} x_2 y_3 + x_3 y_2 \\ x_1 y_3 + x_3 y_1 \\ x_1 y_2 + x_2 y_1 \end{pmatrix}, \tag{1.10d}$$

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{3}_\mathrm{a}} = \frac{\mathrm{i}}{\sqrt{2}} \begin{pmatrix} x_2 y_3 - x_3 y_2 \\ x_3 y_1 - x_1 y_3 \\ x_1 y_2 - x_2 y_1 \end{pmatrix}, \tag{1.10e}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_j}\right)_{\mathbf{1}_{i+j}} = \frac{-1}{\sqrt{2}} \left(\psi_1 \chi_2 - \psi_2 \chi_1\right), \tag{1.10f}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{3-i}}\right)_{\mathbf{3}} = \frac{1}{\sqrt{3}} \begin{pmatrix} -\psi_1\chi_1 + \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \psi_2 \chi_2 \\ -\omega\, \psi_1\chi_1 + \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \omega^2\, \psi_2 \chi_2 \\ -\omega^2\, \psi_1\chi_1 + \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \omega\, \psi_2 \chi_2 \end{pmatrix}, \tag{1.10g}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{2-i}}\right)_{\mathbf{3}} = \frac{1}{\sqrt{3}} \begin{pmatrix} -\psi_1\chi_1 + \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \psi_2 \chi_2 \\ -\psi_1\chi_1 + \omega^2\, \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \omega\, \psi_2 \chi_2 \\ -\psi_1\chi_1 + \omega\, \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \omega^2\, \psi_2 \chi_2 \end{pmatrix}, \tag{1.10h}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{1-i}}\right)_{\mathbf{3}} = \frac{1}{\sqrt{3}} \begin{pmatrix} -\psi_1\chi_1 + \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \psi_2 \chi_2 \\ -\omega^2\, \psi_1\chi_1 + \omega\, \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \psi_2 \chi_2 \\ -\omega\, \psi_1\chi_1 + \omega^2\, \frac{1}{\sqrt{2}} \left(\psi_1 \chi_2 + \psi_2 \chi_1\right) + \psi_2 \chi_2 \end{pmatrix}, \tag{1.10i}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_i} = \frac{1}{3} \begin{pmatrix} \psi_1 \left(x_1 + x_2 + x_3\right) + \sqrt{2}\, \psi_2 \left(x_1 + \omega^2 x_2 + \omega x_3\right) \\ \sqrt{2}\, \psi_1 \left(x_1 + \omega x_2 + \omega^2 x_3\right) - \psi_2 \left(x_1 + x_2 + x_3\right) \end{pmatrix}, \tag{1.10j}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_{i+1}} = \frac{1}{3} \begin{pmatrix} \psi_1 \left(x_1 + \omega^2 x_2 + \omega x_3\right) + \sqrt{2}\, \psi_2 \left(x_1 + \omega x_2 + \omega^2 x_3\right) \\ \sqrt{2}\, \psi_1 \left(x_1 + x_2 + x_3\right) - \psi_2 \left(x_1 + \omega^2 x_2 + \omega x_3\right) \end{pmatrix}, \tag{1.10k}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_{i+2}} = \frac{1}{3} \begin{pmatrix} \psi_1 \left(x_1 + \omega x_2 + \omega^2 x_3\right) + \sqrt{2}\, \psi_2 \left(x_1 + x_2 + x_3\right) \\ \sqrt{2}\, \psi_1 \left(x_1 + \omega^2 x_2 + \omega x_3\right) - \psi_2 \left(x_1 + \omega x_2 + \omega^2 x_3\right) \end{pmatrix}. \tag{1.10l}$$

Ishimori et al. basis

Another basis for T′ was provided by Ishimori et al. [57]. It uses

$$\rho^{\mathrm{I}}_{\mathbf{2}_i}(s) = -\frac{1}{\sqrt{3}}\begin{pmatrix} \mathrm{i} & \sqrt{2}\,p \\ -\sqrt{2}\,p^* & -\mathrm{i} \end{pmatrix}, \qquad i = 0,\,1,\,2\,, \tag{1.11a}$$

$$\rho^{\mathrm{I}}_{\mathbf{2}_0}(t) = \begin{pmatrix} \omega^2 & 0 \\ 0 & \omega \end{pmatrix}, \qquad \rho^{\mathrm{I}}_{\mathbf{2}_1}(t) = \begin{pmatrix} 1 & 0 \\ 0 & \omega^2 \end{pmatrix}, \qquad \rho^{\mathrm{I}}_{\mathbf{2}_2}(t) = \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix}, \tag{1.11b}$$

$$\rho^{\mathrm{I}}_{\mathbf{3}}(s) = \begin{pmatrix} -1 & 2\,p_1 & 2\,p_1\,p_2 \\ 2\,p_1^* & -1 & 2p_2 \\ 2\,p_1^*\,p_2^* & 2\,p_2^* & -1 \end{pmatrix}, \qquad \rho^{\mathrm{I}}_{\mathbf{3}}(s) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix} \tag{1.11c}$$

as generators with $p = \mathrm{e}^{\mathrm{i}\,\phi}$, $p_1 = \mathrm{e}^{\mathrm{i}\,\phi_1}$, and $p_2 = \mathrm{e}^{\mathrm{i}\,\phi_2}$, where ϕ, ϕ_1, and ϕ_2 are arbitrary real phases. The free phases of the triplet representation can be removed by a transformation $\rho^{\mathrm{I}'}_{\mathbf{3}}(s) = P\,\rho^{\mathrm{I}}_{\mathbf{3}}(s)\,P^\dagger$ with

$$P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\,\phi_1} & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}(\phi_1+\phi_2)} \end{pmatrix}. \tag{1.12}$$

The transformation which connects the bases (1.9) and (1.11) for the triplet representations is given by

$$\rho^{\mathrm{M}}_{\mathbf{3}}(s) = (U_\omega\,P)\,\rho^{\mathrm{I}}_{\mathbf{3}}(s)\,(U_\omega\,P)^\dagger \qquad \text{and} \qquad \rho^{\mathrm{M}}_{\mathbf{3}}(t) = (U_\omega\,P)\,\rho^{\mathrm{I}}_{\mathbf{3}}(t)\,(U_\omega\,P)^\dagger, \tag{1.13}$$

with U_ω as defined for A_4 in (1.5).

Note that for the particular choice of $p = \mathrm{i}$ and $p_1 = p_2 = 1$, the representation matrices of basis (1.11) fulfil the Bickerstaff–Damhus condition (VII.5.1) for the automorphism

$$u: \quad (s,t) \quad \mapsto \quad (s^3, t^2)\ . \tag{1.14}$$

Hence, in this particular basis, all Clebsch–Gordan coefficients are real, i.e. the basis is a CP basis. This has also been found in an explicit computation in [57]. The explicit expressions for the tensor products in the CP basis are:

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{1}_0} = \frac{x_1\,y_1 + x_2\,y_3 + x_3\,y_2}{\sqrt{3}}, \tag{1.15a}$$

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{1}_1} = \frac{x_1\,y_2 + x_2\,y_1 + x_3\,y_3}{\sqrt{3}}, \tag{1.15b}$$

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{1}_2} = \frac{x_1\,y_3 + x_2\,y_2 + x_3\,y_1}{\sqrt{3}}, \tag{1.15c}$$

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{3}_\mathrm{s}} = \frac{1}{\sqrt{6}}\begin{pmatrix} 2x_1\,y_1 - x_3\,y_2 - x_2\,y_3 \\ -x_2\,y_1 - x_1\,y_2 + 2x_3\,y_3 \\ -x_3\,y_1 + 2x_2\,y_2 - x_1\,y_3 \end{pmatrix}, \tag{1.15d}$$

$$(x_{\mathbf{3}} \otimes y_{\mathbf{3}})_{\mathbf{3}_\mathrm{a}} = \frac{1}{\sqrt{2}}\begin{pmatrix} x_2\,y_3 - x_3\,y_2 \\ x_1\,y_2 - x_2\,y_1 \\ x_3\,y_1 - x_1\,y_3 \end{pmatrix}, \tag{1.15e}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_j}\right)_{\mathbf{1}_{i+j}} = \frac{\psi_2\,\chi_1 - \psi_1\,\chi_2}{\sqrt{2}}, \tag{1.15f}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{3-i}}\right)_{\mathbf{3}} = \begin{pmatrix} \frac{1}{\sqrt{2}}\left(\psi_1 \chi_2 + \psi_2 \chi_1\right) \\ -\psi_1 \chi_1 \\ \psi_2 \chi_2 \end{pmatrix}, \tag{1.15g}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{2-i}}\right)_{\mathbf{3}} = \begin{pmatrix} -\psi_1 \chi_1 \\ \psi_2 \chi_2 \\ \frac{1}{\sqrt{2}}\left(\psi_1 \chi_2 + \psi_2 \chi_1\right) \end{pmatrix}, \tag{1.15h}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{1-i}}\right)_{\mathbf{3}} = \begin{pmatrix} \psi_2 \chi_2 \\ \frac{1}{\sqrt{2}}\left(\psi_1 \chi_2 + \psi_2 \chi_1\right) \\ -\psi_1 \chi_1 \end{pmatrix}, \tag{1.15i}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_i} = \frac{1}{\sqrt{3}} \begin{pmatrix} \psi_1 \chi_1 + \sqrt{2}\, \psi_2 \chi_2 \\ \sqrt{2}\, \psi_1 \chi_3 - \psi_2 \chi_1 \end{pmatrix}, \tag{1.15j}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_{i+1}} = \frac{1}{\sqrt{3}} \begin{pmatrix} \psi_1 \chi_2 + \sqrt{2}\, \psi_2 \chi_3 \\ \sqrt{2}\, \psi_1 \chi_1 - \psi_2 \chi_2 \end{pmatrix}, \tag{1.15k}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_{i+2}} = \frac{1}{\sqrt{3}} \begin{pmatrix} \psi_1 \chi_3 + \sqrt{2}\, \psi_2 \chi_1 \\ \sqrt{2}\, \psi_1 \chi_2 - \psi_2 \chi_3 \end{pmatrix}. \tag{1.15l}$$

Another basis commonly used in the literature is the one of Feruglio et al. [26, Appendix A], which can be obtained from (1.11) by setting $p_1 = p_2 = \mathrm{e}^{2\pi\,\mathrm{i}\,/3}$ and $p = \mathrm{e}^{2\pi\,\mathrm{i}\,/24}$. Note that their phases do not coincide with the ones obtained by a basis transformation from the CP basis. With the phases obtained by the basis transformation, which are then such that compounds transform like elementary states, the component expressions of the Clebsch–Gordan coefficients are

$$\left(x_{\mathbf{3}} \otimes y_{\mathbf{3}}\right)_{\mathbf{1}_0} = \frac{x_1 y_1 + x_2 y_3 + x_3 y_2}{\sqrt{3}}, \tag{1.16a}$$

$$\left(x_{\mathbf{3}} \otimes y_{\mathbf{3}}\right)_{\mathbf{1}_1} = \frac{\omega\left(x_1 y_2 + x_2 y_1 + x_3 y_3\right)}{\sqrt{3}}, \tag{1.16b}$$

$$\left(x_{\mathbf{3}} \otimes y_{\mathbf{3}}\right)_{\mathbf{1}_2} = \frac{\omega^2\left(x_1 y_3 + x_2 y_2 + x_3 y_1\right)}{\sqrt{3}}, \tag{1.16c}$$

$$\left(x_{\mathbf{3}} \otimes y_{\mathbf{3}}\right)_{\mathbf{3}_\mathrm{s}} = \frac{1}{\sqrt{6}} \begin{pmatrix} 2x_1 y_1 - x_3 y_2 - x_2 y_3 \\ -x_2 y_1 - x_1 y_2 + 2x_3 y_3 \\ -x_3 y_1 + 2x_2 y_2 - x_1 y_3 \end{pmatrix}, \tag{1.16d}$$

$$\left(x_{\mathbf{3}} \otimes y_{\mathbf{3}}\right)_{\mathbf{3}_\mathrm{a}} = \frac{1}{\sqrt{2}} \begin{pmatrix} x_2 y_3 - x_3 y_2 \\ x_1 y_2 - x_2 y_1 \\ x_3 y_1 - x_1 y_3 \end{pmatrix}, \tag{1.16e}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_j}\right)_{\mathbf{1}_{i+j}} = \frac{\mathrm{e}^{7\,\mathrm{i}\,\pi/12}}{\sqrt{2}}\left(\psi_1 \chi_2 - \psi_2 \chi_1\right), \tag{1.16f}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{3-i}}\right)_{\mathbf{3}} = \mathrm{i}\,\omega^2 \begin{pmatrix} \frac{1-\mathrm{i}}{2}\left(\psi_1 \chi_2 + \psi_2 \chi_1\right) \\ \mathrm{i}\ \psi_1 \chi_1 \\ \psi_2 \chi_2 \end{pmatrix}, \tag{1.16g}$$

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{2-i}}\right)_{\mathbf{3}} = \mathrm{i} \begin{pmatrix} \mathrm{i}\,\psi_1 \chi_1 \\ \psi_2 \chi_2 \\ \frac{1-\mathrm{i}}{2}\left(\psi_1 \chi_2 + \psi_2 \chi_1\right) \end{pmatrix}, \tag{1.16h}$$

	C_{1a}	C_{3a}	C_{3b}	C_{3c}	C_{3d}	C_{3e}	C_{3f}	C_{3g}	C_{3h}	C_{3i}	C_{3j}
	1	3	3	3	3	3	3	3	3	1	1
$\Delta(27)$	e	a	a^2	b	b^2	aba	bab	ab	a^2b^2	ab^2aba	ba^2bab
$\mathbf{1}_0$	1	1	1	1	1	1	1	1	1	1	1
$\mathbf{1}_1$	1	1	1	ω^2	ω	ω^2	ω	ω^2	ω	1	1
$\mathbf{1}_2$	1	1	1	ω	ω^2	ω	ω^2	ω	ω^2	1	1
$\mathbf{1}_3$	1	ω^2	ω	1	1	ω	ω^2	ω^2	ω	1	1
$\mathbf{1}_4$	1	ω^2	ω	ω^2	ω	1	1	ω	ω^2	1	1
$\mathbf{1}_5$	1	ω^2	ω	ω	ω^2	ω^2	ω	1	1	1	1
$\mathbf{1}_6$	1	ω	ω^2	1	1	ω^2	ω	ω	ω^2	1	1
$\mathbf{1}_7$	1	ω	ω^2	ω^2	ω	ω	ω^2	1	1	1	1
$\mathbf{1}_8$	1	ω	ω^2	ω	ω^2	1	1	ω^2	ω	1	1
$\mathbf{3}$	3	0	0	0	0	0	0	0	0	$3\omega^2$	3ω
$\overline{\mathbf{3}}$	3	0	0	0	0	0	0	0	0	3ω	$3\omega^2$

Table A.3: Character table of $\Delta(27)$, where $\omega := \mathrm{e}^{2\pi\,\mathrm{i}\,/3}$.

$$\left(\psi_{\mathbf{2}_i} \otimes \chi_{\mathbf{2}_{1-i}}\right)_{\mathbf{3}} = \mathrm{i}\,\omega \begin{pmatrix} \psi_2 \chi_2 \\ \frac{1-\mathrm{i}}{2}\,(\psi_1 \chi_2 + \psi_2 \chi_1) \\ \mathrm{i}\,\psi_1 \chi_1 \end{pmatrix}, \tag{1.16i}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_i} = \frac{1}{\sqrt{3}} \begin{pmatrix} \psi_1 \chi_1 + (1+\mathrm{i})\,\psi_2 \chi_2 \\ (1-\mathrm{i})\,\psi_1 \chi_3 - \psi_2 \chi_1 \end{pmatrix}, \tag{1.16j}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_{i+1}} = \frac{\omega}{\sqrt{3}} \begin{pmatrix} (\psi_1 \chi_2 + (1+\mathrm{i})\,\psi_2 \chi_3) \\ (1-\mathrm{i})\,\psi_1 \chi_1 - \psi_2 \chi_2 \end{pmatrix}, \tag{1.16k}$$

$$\left(\psi_{\mathbf{2}_i} \otimes x_{\mathbf{3}}\right)_{\mathbf{2}_{i+2}} = \frac{\omega^2}{\sqrt{3}} \begin{pmatrix} \psi_1 \chi_3 + (1+\mathrm{i})\,\psi_2 \chi_1 \\ (1-\mathrm{i})\,\psi_1 \chi_2 - \psi_2 \chi_3 \end{pmatrix}. \tag{1.16l}$$

A.1.3 The group $\Delta(27)$

The group $\Delta(27)$ is a subgroup of SU(3) and an element of the infinite SU(3) subgroup family $\Delta(3 \cdot n^2)$. It is generated by two elements a and b fulfilling the relations

$$a^3 = b^3 = (ab)^3 = e\,. \tag{1.17}$$

There are eleven inequivalent irreducible representations: $\mathbf{1}_i$, where $i = 0, \ldots, 8$, $\mathbf{3}$ and $\overline{\mathbf{3}}$. The character table is shown as Table A.3.

We adopt the labelling of [15] with the difference that in our notation $\mathbf{1}_i = \mathbf{1}_{i-1}^{(\mathrm{HLS})}$ and use the contractions of [219] translated to our conventions. The representations in the pairs $(\mathbf{1}_1, \mathbf{1}_2)$, $(\mathbf{1}_3, \mathbf{1}_6)$, $(\mathbf{1}_4, \mathbf{1}_8)$, and $(\mathbf{1}_5, \mathbf{1}_7)$ as well as the triplets are complex conjugates of each other. As matrix realisations of the generators in the triplet representation

$$A := \rho_{\mathbf{3}}(a) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \tag{1.18a}$$

$$B := \rho_{\mathbf{3}}(b) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix} \tag{1.18b}$$

are chosen and for $\overline{\mathbf{3}}$ the corresponding complex conjugate matrices.

The tensor product of a triplet and an anti-triplet yields a complete set of singlets,

$$\mathbf{3} \otimes \overline{\mathbf{3}} \cong \bigoplus_{i=1}^{9} \mathbf{1}_i \,. \tag{1.19}$$

The expressions of the singlet components in the tensor product of the triplet x with the anti-triplet y read

$$\mathbf{1}_0 = \frac{(x_1 y_1 + x_2 y_2 + x_3 y_3)}{\sqrt{3}}\,, \tag{1.20a}$$

$$\mathbf{1}_1 = \frac{(x_1 y_2 + x_2 y_3 + x_3 y_1)}{\sqrt{3}}\,, \qquad \mathbf{1}_2 = \frac{(x_2 y_1 + x_3 y_2 + x_1 y_3)}{\sqrt{3}}\,, \tag{1.20b}$$

$$\mathbf{1}_3 = \frac{(x_1 y_1 + \omega x_2 y_2 + \omega^2 x_3 y_3)}{\sqrt{3}}\,, \qquad \mathbf{1}_6 = \frac{(x_1 y_1 + \omega^2 x_2 y_2 + \omega x_3 y_3)}{\sqrt{3}}\,, \tag{1.20c}$$

$$\mathbf{1}_4 = \frac{(x_1 y_2 + \omega x_2 y_3 + \omega^2 x_3 y_1)}{\sqrt{3}}\,, \qquad \mathbf{1}_8 = \frac{(x_2 y_1 + \omega^2 x_3 y_2 + \omega x_1 y_3)}{\sqrt{3}}\,, \tag{1.20d}$$

$$\mathbf{1}_5 = \frac{(x_2 y_1 + \omega x_3 y_2 + \omega^2 x_1 y_3)}{\sqrt{3}}\,, \qquad \mathbf{1}_7 = \frac{(x_1 y_2 + \omega^2 x_2 y_3 + \omega x_3 y_1)}{\sqrt{3}}\,. \tag{1.20e}$$

As a non-abelian group of odd order, i.e. with an odd number of elements, $\Delta(27)$ cannot have a class-inverting automorphism. However, there are in total 46 involutory automorphisms, which interchange some representations with their complex conjugates. For example

$$u_1 : \quad (a,b) \mapsto (a,b^2) \qquad \Rightarrow \mathbf{1}_1 \leftrightarrow \mathbf{1}_2\,,\ \mathbf{1}_4 \leftrightarrow \mathbf{1}_5\,,\ \mathbf{1}_7 \leftrightarrow \mathbf{1}_8\,,\ \mathbf{3} \to U_{u_1}\overline{\mathbf{3}}\,, \tag{1.21a}$$

$$u_2 : \quad (a,b) \mapsto (aba,b) \qquad \Rightarrow \mathbf{1}_1 \leftrightarrow \mathbf{1}_4\,,\ \mathbf{1}_2 \leftrightarrow \mathbf{1}_8\,,\ \mathbf{1}_3 \leftrightarrow \mathbf{1}_6\,,\ \mathbf{3} \to U_{u_2}\overline{\mathbf{3}}\,, \tag{1.21b}$$

$$u_3 : \quad (a,b) \mapsto (bab,b^2) \qquad \Rightarrow \mathbf{1}_1 \leftrightarrow \mathbf{1}_8\,,\ \mathbf{1}_2 \leftrightarrow \mathbf{1}_4\,,\ \mathbf{1}_5 \leftrightarrow \mathbf{1}_7\,,\ \mathbf{3} \to U_{u_3}\overline{\mathbf{3}}\,, \tag{1.21c}$$

$$u_4 : \quad (a,b) \mapsto (ab^2a,b) \qquad \Rightarrow \mathbf{1}_1 \leftrightarrow \mathbf{1}_7\,,\ \mathbf{1}_2 \leftrightarrow \mathbf{1}_5\,,\ \mathbf{1}_3 \leftrightarrow \mathbf{1}_6\,,\ \mathbf{3} \to U_{u_4}\overline{\mathbf{3}}\,, \tag{1.21d}$$

$$u_5 : \quad (a,b) \mapsto (ba^2b^2, ab^2a^2) \qquad \Rightarrow \mathbf{1}_i \leftrightarrow \overline{\mathbf{1}}_i\,,\ \mathbf{3} \to U_{u_5}\mathbf{3}\,. \tag{1.21e}$$

Any representation not listed is mapped to itself under the respective automorphism. $\mathbf{3} \to U_{u_i}\overline{\mathbf{3}}$ means that fields in the triplet representation have to be multiplied by the corresponding matrix in addition to the conjugation. In the basis defined above, these matrices are

$$U_{u_1} = \mathbb{1}\,, \qquad U_{u_2} = \begin{pmatrix} \omega & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad U_{u_3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega^2 & 0 \\ 0 & 0 & \omega^2 \end{pmatrix},$$

$$U_{u_4} = \begin{pmatrix} \omega^2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad U_{u_5} = \begin{pmatrix} 0 & 0 & \omega^2 \\ 0 & 1 & 0 \\ \omega & 0 & 0 \end{pmatrix}. \tag{1.22}$$

The corresponding twisted Frobenius–Schur indicators for all representations are given in Table A.4. One can convince oneself by computing the twisted Frobenius–Schur indicators for all automorphisms of $\Delta(27)$ that for models with fields in more than two different, non-conjugate non-trivial one-dimensional representations and a triplet it is impossible to define a consistent CP transformation.

	$\mathbf{1}_0$	$\mathbf{1}_1$	$\mathbf{1}_2$	$\mathbf{1}_3$	$\mathbf{1}_4$	$\mathbf{1}_5$	$\mathbf{1}_6$	$\mathbf{1}_7$	$\mathbf{1}_8$	$\mathbf{3}$	$\overline{\mathbf{3}}$
FS_{u_1}	1	1	1	0	0	0	0	0	0	1	1
FS_{u_2}	1	0	0	1	0	0	1	0	0	1	1
FS_{u_3}	1	0	0	0	0	1	0	1	0	1	1
FS_{u_4}	1	0	0	1	0	0	1	0	0	1	1
FS_{u_5}	1	1	1	1	1	1	1	1	1	0	0

Table A.4: Twisted Frobenius–Schur indicators for some $\Delta(27)$ automorphisms.

	C_{1a}	C_{3a}	C_{3b}	C_{3c}	C_{3d}	C_{2a}	C_{6a}	C_{6b}	C_{3e}	C_{3f}
	1	6	6	6	6	9	9	9	1	1
$\Delta(54)$	e	a	b	aba	ab	c	abc	bac	ab^2aba	ba^2bab
$\mathbf{1}_0$	1	1	1	1	1	1	1	1	1	1
$\mathbf{1}_1$	1	1	1	1	1	−1	−1	−1	1	1
$\mathbf{2}_1$	2	2	−1	−1	−1	0	0	0	2	2
$\mathbf{2}_2$	2	−1	2	−1	−1	0	0	0	2	2
$\mathbf{2}_3$	2	−1	−1	2	−1	0	0	0	2	2
$\mathbf{2}_4$	2	−1	−1	−1	2	0	0	0	2	2
$\mathbf{3}_1$	3	0	0	0	0	1	ω^2	ω	3ω	$3\omega^2$
$\overline{\mathbf{3}}_1$	3	0	0	0	0	1	ω	ω^2	$3\omega^2$	3ω
$\mathbf{3}_2$	3	0	0	0	0	−1	$-\omega^2$	$-\omega$	3ω	$3\omega^2$
$\overline{\mathbf{3}}_2$	3	0	0	0	0	−1	$-\omega$	$-\omega^2$	$3\omega^2$	3ω

Table A.5: Character table of $\Delta(54)$, where $\omega := \mathrm{e}^{2\pi\,\mathrm{i}\,/3}$.

A.1.4 The group $\Delta(54)$

Like $\Delta(27)$, the group $\Delta(54)$ is a subgroup of $\mathrm{SU}(3)$. In fact, it is part of the $\Delta(6 \cdot n^2)$ chain of subgroups and contains $\Delta(27)$ as a normal subgroup. $\Delta(54)$ is generated by three elements a, b, and c, where

$$a^3 = b^3 = c^2 = (ab)^3 = (ac)^2 = (bc)^2 = e\,. \tag{1.23}$$

There are five non-trivial real irreducible representations $\mathbf{1}_1$ and $\mathbf{2}_i$ with $i = 1, \ldots, 4$ and, in addition, the complex representations $\mathbf{3}_1$ and $\mathbf{3}_2$ with their respective conjugates. The characters are shown in Table A.5.

For the triplets $\mathbf{3}_{1,2}$ the representation matrices

$$\rho_{\mathbf{3}_{1,2}}(a) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \rho_{\mathbf{3}_{1,2}}(b) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \qquad \rho_{\mathbf{3}_{1,2}}(c) = \pm \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{1.24}$$

are chosen with the plus sign for $\mathbf{3}_1$. For $\overline{\mathbf{3}}_{1,2}$ the corresponding complex conjugate matrices are used.

Restricting the conjugation map $\mathrm{conj}(c)$ from $\Delta(54)$ to $\Delta(27)$, one obtains a non-inner automorphism of $\Delta(27)$ which exchanges all singlet representations with their respective complex conjugates. The decomposition of the real $\Delta(54)$ doublets into the complex $\Delta(27)$ singlets is thus given by $\mathbf{2}_1 = (\mathbf{1}_1, \mathbf{1}_2)$, $\mathbf{2}_2 = (\mathbf{1}_3, \mathbf{1}_6)$, $\mathbf{2}_3 = (\mathbf{1}_4, \mathbf{1}_8)$ and $\mathbf{2}_4 = (\mathbf{1}_5, \mathbf{1}_7)$.

	C_{1a}	C_{3a}	C_{2a}	C_{4a}	C_{4b}	C_{4c}
	1	8	9	18	18	18
$\Sigma(72)$	e	p	m^2	mn	n	m
$\mathbf{1}_0$	1	1	1	1	1	1
$\mathbf{1}_1$	1	1	1	1	−1	−1
$\mathbf{1}_2$	1	1	1	−1	1	−1
$\mathbf{1}_3$	1	1	1	−1	−1	1
$\mathbf{2}$	2	2	−2	0	0	0
$\mathbf{8}$	8	−1	0	0	0	0

Table A.6: Character table of $\Sigma(72)$.

In a basis where the $\Delta(27)$ subgroup has block-diagonal representation matrices for the doublets, the relevant Clebsch–Gordan coefficients of $\Delta(54)$ are

$$\left(x_{\mathbf{2}_i} \otimes y_{\mathbf{2}_i}\right)_{\mathbf{1}_0} = \frac{1}{\sqrt{2}} \left(x_1 y_2 + x_2 y_1\right) , \tag{1.25a}$$

$$\left(x_{\mathbf{3}_i} \otimes y_{\bar{\mathbf{3}}_i}\right)_{\mathbf{1}_0} = \frac{1}{\sqrt{3}} \left(x_1 y_1 + x_2 y_2 + x_3 y_3\right) , \tag{1.25b}$$

$$\left(x_{\mathbf{3}_i} \otimes y_{\bar{\mathbf{3}}_i}\right)_{\mathbf{2}_1} = \frac{1}{\sqrt{3}} \begin{pmatrix} x_1 y_2 + x_3 y_1 + x_2 y_3 \\ x_2 y_1 + x_1 y_3 + x_3 y_2 \end{pmatrix} , \tag{1.25c}$$

$$\left(x_{\mathbf{3}_i} \otimes y_{\bar{\mathbf{3}}_i}\right)_{\mathbf{2}_2} = \frac{1}{\sqrt{3}} \begin{pmatrix} x_1 y_1 + \omega x_2 y_2 + \omega^2 x_3 y_3 \\ x_1 y_1 + \omega^2 x_2 y_2 + \omega x_3 y_3 \end{pmatrix} , \tag{1.25d}$$

$$\left(x_{\mathbf{3}_i} \otimes y_{\bar{\mathbf{3}}_i}\right)_{\mathbf{2}_3} = \frac{1}{\sqrt{3}} \begin{pmatrix} x_2 y_3 + \omega x_3 y_1 + \omega^2 x_1 y_2 \\ \omega x_2 y_1 + x_3 y_2 + \omega^2 x_1 y_3 \end{pmatrix} , \tag{1.25e}$$

$$\left(x_{\mathbf{3}_i} \otimes y_{\bar{\mathbf{3}}_i}\right)_{\mathbf{2}_4} = \frac{1}{\sqrt{3}} \begin{pmatrix} \omega^2 x_2 y_1 + x_3 y_2 + \omega x_1 y_3 \\ x_2 y_3 + \omega^2 x_3 y_1 + \omega x_1 y_2 \end{pmatrix} . \tag{1.25f}$$

For the other Clebsch–Gordan coefficients, cf. [57].

A.1.5 The group $\Sigma(72)$

The non-abelian group $\Sigma(72)$ is isomorphic to the semi-direct product group $(\mathbb{Z}_3 \times \mathbb{Z}_3) \rtimes Q_8$, where Q_8 is the Quaternion group. It is generated by three generators m, n and p fulfilling the relations

$$\begin{aligned} &m^4 = n^4 = p^3 = \left(m^2 p^{-1}\right)^2 = e\,, \qquad m^2 = n^2\,, \qquad m^{-1} n = n\, m\,, \\ &p\, m\, p\, n^{-1}\, m\, p^{-1}\, n = e\,, \qquad n\, p\, m^{-1}\, p = m\, p\, n\,. \end{aligned} \tag{1.26}$$

$\Sigma(72)$ has 6 inequivalent irreducible representations: four one-dimensional ($\mathbf{1}_{0-3}$), one two-dimensional ($\mathbf{2}$), and one eight–dimensional ($\mathbf{8}$) one. The characters of $\Sigma(72)$ are shown in Table A.6. Since all characters are real, it is clear that $\Sigma(72)$ is ambivalent and that all representations are (pseudo-) real. For the two-dimensional representation, the generators can be chosen as

$$\rho_{\mathbf{2}}(m) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} , \qquad \rho_{\mathbf{2}}(n) = \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix} , \qquad \rho_{\mathbf{2}}(p) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \tag{1.27}$$

and for the eight-dimensional one as

$$\rho_{\mathbf{8}}(m) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \end{pmatrix}, \qquad \rho_{\mathbf{8}}(n) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{1.28a}$$

$$\rho_{\mathbf{8}}(p) = \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\sqrt{3} & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & -\sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{3} & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -\sqrt{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{3} & -1 \end{pmatrix}. \tag{1.28b}$$

For this basis, the non-trivial tensor product contractions of $\Sigma(72)$ are shown in the following.

$$\left(x_{\mathbf{1}_0} \otimes y_{\mathbf{2}}\right)_{\mathbf{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} x_1 y_1 \\ x_1 y_2 \end{pmatrix}, \qquad \left(x_{\mathbf{1}_1} \otimes y_{\mathbf{2}}\right)_{\mathbf{2}} = \frac{\mathrm{i}}{\sqrt{2}} \begin{pmatrix} x_1 y_2 \\ x_1 y_1 \end{pmatrix}, \tag{1.29a}$$

$$\left(x_{\mathbf{1}_2} \otimes y_{\mathbf{2}}\right)_{\mathbf{2}} = \frac{\mathrm{i}}{\sqrt{2}} \begin{pmatrix} x_1 y_1 \\ -x_1 y_2 \end{pmatrix}, \qquad \left(x_{\mathbf{1}_3} \otimes y_{\mathbf{2}}\right)_{\mathbf{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} x_1 y_2 \\ -x_1 y_1 \end{pmatrix}, \tag{1.29b}$$

$$(x_{\mathbf{2}} \otimes y_{\mathbf{2}})_{\mathbf{1}_0} = \frac{1}{\sqrt{2}} (x_1 y_2 - x_2 y_1), \qquad (x_{\mathbf{2}} \otimes y_{\mathbf{2}})_{\mathbf{1}_1} = \frac{\mathrm{i}}{\sqrt{2}} (x_1 y_1 - x_2 y_2), \tag{1.29c}$$

$$(x_{\mathbf{2}} \otimes y_{\mathbf{2}})_{\mathbf{1}_2} = \frac{\mathrm{i}}{\sqrt{2}} (x_1 y_2 + x_2 y_1), \qquad (x_{\mathbf{2}} \otimes y_{\mathbf{2}})_{\mathbf{1}_3} = \frac{1}{\sqrt{2}} (x_1 y_1 + x_2 y_2), \tag{1.29d}$$

$$\left(x_{\mathbf{1}_0} \otimes y_{\mathbf{8}}\right)_{\mathbf{8}} = (x_1 y_1, x_1 y_2, x_1 y_3, x_1 y_4, x_1 y_5, x_1 y_6, x_1 y_7, x_1 y_8)^T, \tag{1.29e}$$

$$\left(x_{\mathbf{1}_1} \otimes y_{\mathbf{8}}\right)_{\mathbf{8}} = (x_1 y_1, x_1 y_2, -x_1 y_3, -x_1 y_4, -x_1 y_5, -x_1 y_6, x_1 y_7, x_1 y_8)^T, \tag{1.29f}$$

$$\left(x_{\mathbf{1}_2} \otimes y_{\mathbf{8}}\right)_{\mathbf{8}} = (x_1 y_1, x_1 y_2, -x_1 y_3, -x_1 y_4, x_1 y_5, x_1 y_6, -x_1 y_7, -x_1 y_8)^T, \tag{1.29g}$$

$$\left(x_{\mathbf{1}_3} \otimes y_{\mathbf{8}}\right)_{\mathbf{8}} = (x_1 y_1, x_1 y_2, x_1 y_3, x_1 y_4, -x_1 y_5, -x_1 y_6, -x_1 y_7, -x_1 y_8)^T, \tag{1.29h}$$

$$(x_{\mathbf{2}} \otimes y_{\mathbf{8}})_{\mathbf{8}^1} = (\mathrm{i}\, x_1 y_2, -\mathrm{i}\, x_1 y_1, \mathrm{i}\, x_2 y_4, -\mathrm{i}\, x_2 y_3, x_1 y_6, -x_1 y_5, x_2 y_8, -x_2 y_7)^T, \tag{1.29i}$$

$$(x_{\mathbf{2}} \otimes y_{\mathbf{8}})_{\mathbf{8}^2} = (\mathrm{i}\, x_2 y_2, -\mathrm{i}\, x_2 y_1, -\mathrm{i}\, x_1 y_4, \mathrm{i}\, x_1 y_3, -x_2 y_6, x_2 y_5, x_1 y_8, -x_1 y_7)^T, \tag{1.29j}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{1}_0} = \frac{1}{2\sqrt{2}} (x_1 y_1 + x_2 y_2 + x_3 y_3 + x_4 y_4 + x_5 y_5 + x_6 y_6 + x_7 y_7 + x_8 y_8), \tag{1.29k}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{1}_1} = \frac{1}{2\sqrt{2}} \left(x_1 y_1 + x_2 y_2 - x_3 y_3 - x_4 y_4 - x_5 y_5 - x_6 y_6 + x_7 y_7 + x_8 y_8\right) , \tag{1.29l}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{1}_2} = \frac{1}{2\sqrt{2}} \left(x_1 y_1 + x_2 y_2 - x_3 y_3 - x_4 y_4 + x_5 y_5 + x_6 y_6 - x_7 y_7 - x_8 y_8\right) , \tag{1.29m}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{1}_3} = \frac{1}{2\sqrt{2}} \left(x_1 y_1 + x_2 y_2 + x_3 y_3 + x_4 y_4 - x_5 y_5 - x_6 y_6 - x_7 y_7 - x_8 y_8\right) , \tag{1.29n}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{2}^1} = \frac{1}{2} \begin{pmatrix} \mathrm{i}\, x_2 y_1 - \mathrm{i}\, x_1 y_2 - x_6 y_5 + x_5 y_6 \\ \mathrm{i}\, x_4 y_3 - \mathrm{i}\, x_3 y_4 - x_8 y_7 + x_7 y_8 \end{pmatrix} , \tag{1.29o}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{2}^2} = \frac{1}{2} \begin{pmatrix} \mathrm{i}\, x_4 y_3 - \mathrm{i}\, x_3 y_4 + x_8 y_7 - x_7 y_8 \\ -\mathrm{i}\, x_2 y_1 + \mathrm{i}\, x_1 y_2 - x_6 y_5 + x_5 y_6 \end{pmatrix} , \tag{1.29p}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{8}^1} = \frac{1}{\sqrt{2}} \left(x_1 y_1 - x_2 y_2,\, -x_2 y_1 - x_1 y_2,\, x_3 y_3 - x_4 y_4,\, -x_4 y_3 - x_3 y_4,\right.$$
$$\left. x_5 y_5 - x_6 y_6,\, -x_6 y_5 - x_5 y_6,\, x_7 y_7 - x_8 y_8,\, -x_8 y_7 - x_7 y_8\right)^T , \tag{1.29q}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{8}^2} = \frac{1}{\sqrt{2}} \left(x_3 y_5 + x_4 y_6,\, x_4 y_5 - x_3 y_6,\, x_1 y_7 - x_2 y_8,\, -x_2 y_7 - x_1 y_8,\right.$$
$$\left. x_7 y_1 + x_8 y_2,\, -x_8 y_1 + x_7 y_2,\, x_5 y_3 - x_6 y_4,\, x_6 y_3 + x_5 y_4\right)^T , \tag{1.29r}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{8}^3} = \frac{1}{\sqrt{2}} \left(x_3 y_7 - x_4 y_8,\, -x_4 y_7 - x_3 y_8,\, x_1 y_5 - x_2 y_6,\, x_2 y_5 + x_1 y_6,\right.$$
$$\left. x_7 y_3 + x_8 y_4,\, x_8 y_3 - x_7 y_4,\, x_5 y_1 + x_6 y_2,\, -x_6 y_1 + x_5 y_2\right)^T , \tag{1.29s}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{8}^4} = \frac{1}{\sqrt{2}} \left(x_5 y_7 - x_6 y_8,\, x_6 y_7 + x_5 y_8,\, x_7 y_5 + x_8 y_6,\, x_8 y_5 - x_7 y_6,\right.$$
$$\left. x_1 y_3 + x_2 y_4,\, -x_2 y_3 + x_1 y_4,\, x_3 y_1 - x_4 y_2,\, -x_4 y_1 - x_3 y_2\right)^T , \tag{1.29t}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{8}^5} = \frac{1}{\sqrt{2}} \left(x_5 y_3 + x_6 y_4,\, -x_6 y_3 + x_5 y_4,\, x_7 y_1 - x_8 y_2,\, -x_8 y_1 - x_7 y_2,\right.$$
$$\left. x_1 y_7 + x_2 y_8,\, x_2 y_7 - x_1 y_8,\, x_3 y_5 - x_4 y_6,\, x_4 y_5 + x_3 y_6\right)^T , \tag{1.29u}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{8}^6} = \frac{1}{\sqrt{2}} \left(x_7 y_5 - x_8 y_6,\, x_8 y_5 + x_7 y_6,\, x_5 y_7 + x_6 y_8,\, -x_6 y_7 + x_5 y_8,\right.$$
$$\left. x_3 y_1 + x_4 y_2,\, x_4 y_1 - x_3 y_2,\, x_1 y_3 - x_2 y_4,\, -x_2 y_3 - x_1 y_4\right)^T , \tag{1.29v}$$

$$(x_{\mathbf{8}} \otimes y_{\mathbf{8}})_{\mathbf{8}^7} = \frac{1}{\sqrt{2}} \left(x_7 y_3 - x_8 y_4,\, -x_8 y_3 - x_7 y_4,\, x_5 y_1 - x_6 y_2,\, x_6 y_1 + x_5 y_2,\right.$$
$$\left. x_3 y_7 + x_4 y_8,\, -x_4 y_7 + x_3 y_8,\, x_1 y_5 + x_2 y_6,\, x_2 y_5 - x_1 y_6\right)^T . \tag{1.29w}$$

A.2 Non-real bases for real representations

As detailed in Section II.5, one distinguishes between complex, real and pseudo-real representations. Real representations are representations which are equivalent to their conjugate representation (see Definition 18), $\boldsymbol{R} \cong \overline{\boldsymbol{R}}$, and which can be realised as manifestly real matrices. However, one can, of course, also choose a basis with non-real entries. This can be desirable, for example, if the CP basis, i.e. the basis with real Clebsch–Gordan coefficients, happens to be of this type. An example for this is the CP basis of T′ with its triplet representation, see Section VII.9.1 and Section A.1.2. In this case $\rho_{\boldsymbol{R}}(g)^* \neq \rho_{\boldsymbol{R}}(g)$ for some g in G. For pseudo-real representations this is always the case because they can, by definition, not be represented by real matrices. Moreover, one can choose for a complex representation $\boldsymbol{R}$ and its conjugate $\overline{\boldsymbol{R}}$ two bases such that the representation matrices are not mutually complex conjugate, i.e. $\rho_{\boldsymbol{R}}(g)^* \neq \rho_{\overline{\boldsymbol{R}}}(g)$ for some g in G. Let for the rest of this section $\boldsymbol{R}$ denote a fixed basis for this representation, i.e. not only up to equivalence, and $\overline{\boldsymbol{R}}$ analogously for the conjugate representation. Further, let $\boldsymbol{R}^*$ denote the representation which is defined by complex conjugating all matrices of $\boldsymbol{R}$.

Then the conjugate φ^* of a field φ in representation $\boldsymbol{R}$ does not transform with the representation matrices $\rho_{\overline{\boldsymbol{R}}}$ chosen for the conjugate representation but with $\rho_{\boldsymbol{R}}^*$. However, one usually only computes the Clebsch–Gordan coefficients for tensor products in terms of $\overline{\boldsymbol{R}}$ and not additionally for $\boldsymbol{R}^*$. Using naively the Clebsch–Gordan coefficients of $\boldsymbol{R} \otimes \overline{\boldsymbol{R}}$ for the contraction of φ with φ^*, which actually is $\boldsymbol{R} \otimes \boldsymbol{R}^*$, leads to wrong results. Let φ be in the triplet representation of T′ in the CP basis, for example. Then the contraction of φ and φ^* to the trivial singlet is, as usual,

$$(\varphi^* \otimes \varphi)_{\mathbf{1}_0} = \varphi^\dagger \varphi \,. \tag{2.1}$$

Applying naively the Clebsch–Gordan coefficient of (1.15a), one could be tricked to think that

$$(\varphi^* \otimes \varphi)_{\mathbf{1}_0} = \frac{\varphi_1^* \varphi_1 + \varphi_2^* \varphi_3 + \varphi_3^* \varphi_2}{\sqrt{3}} \tag{2.2}$$

were, up to normalisation, the correct result, which is clearly wrong.

This shows that one has to be careful when using the Clebsch–Gordan coefficients in this special case. As $\overline{\boldsymbol{R}} \cong \boldsymbol{R}^*$, there is a unitary matrix U, unique up to a phase for irreducible $\boldsymbol{R}$, such that

$$\rho_{\overline{\boldsymbol{R}}}(g) = U \rho_{\boldsymbol{R}^*}(g) U^{-1} = U \rho_{\boldsymbol{R}}(g)^* U^{-1} \,. \tag{2.3}$$

With this matrix, one can define the field

$$\bar{\varphi} := U \varphi^* \,, \tag{2.4}$$

which transforms with matrices $\rho_{\overline{\boldsymbol{R}}}$ instead of $\rho_{\boldsymbol{R}}^*$. Hence, using the field $\bar{\varphi}$ instead of φ^*, one can use the Clebsch–Gordan coefficients for $\boldsymbol{R}$ and $\overline{\boldsymbol{R}}$. Taking again the example of the T′ triplet in the CP basis, the matrix U is

$$U := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{2.5}$$

and the contraction reads

$$(\bar{\varphi} \otimes \varphi)_{\mathbf{1}_0} = \frac{\bar{\varphi}_1 \varphi_1 + \bar{\varphi}_2 \varphi_3 + \bar{\varphi}_3 \varphi_2}{\sqrt{3}} = \frac{\varphi_1^* \varphi_1 + \varphi_2^* \varphi_2 + \varphi_3^* \varphi_3}{\sqrt{3}}\,, \tag{2.6}$$

which is the correct result.

The occurrence of the matrix U does not spoil the good CP behaviour in the CP basis because U is always real for real Clebsch–Gordan coefficients. This can be seen from the fact that the trivial singlet contraction of φ and φ^*, which for unitary representations is always $\varphi^\dagger \varphi$ up to a complex normalisation, reads using the Clebsch–Gordan coefficients

$$\bar{\varphi}_a C_{ab,\mathbf{1}_0} \varphi_b = U_{ia} \varphi_a^* C_{ib,\mathbf{1}_0} \varphi_b = \alpha \varphi_a^* \delta_{ab} \varphi_b\,, \tag{2.7}$$

where α is some complex number.[1] The complex phase of α can always be removed by a different choice of U because U is only defined up to a phase. Hence,

$$C_{ib,\mathbf{1}_0} U_{ia} = |\alpha| \delta_{ab}\,, \tag{2.8}$$

i.e. U is the inverse of a matrix with real coefficients and, therefore, real itself.

A.2.1 Real scalar fields in not manifestly real representations

Related issues can arise for a field φ transforming in a real representation $\boldsymbol{R}$ with not manifestly real representation matrices.[2] Starting with a real matrix realisation $\rho_{\boldsymbol{R}}$ of $\boldsymbol{R}$,

$$\rho_{\boldsymbol{R}}(g) = \rho_{\boldsymbol{R}}(g)^*\,, \qquad \forall\, g \in G\,, \tag{2.9}$$

one can consistently impose the reality condition

$$\varphi = \varphi^* \tag{2.10}$$

on the field.

Let us now change to a different matrix realisation of $\boldsymbol{R}$,

$$\varphi' = S^{-1} \varphi\,, \tag{2.11a}$$
$$\rho'_{\boldsymbol{R}}(g) = S^{-1} \rho_{\boldsymbol{R}}(g)\, S\,, \tag{2.11b}$$

where S is a unitary matrix, and study the theory in this new basis. In contrast to $\rho_{\boldsymbol{R}}(g)$, the matrix realisation $\rho'_{\boldsymbol{R}}(g)$ need not be manifestly real. In fact,

$$\rho'_{\boldsymbol{R}}(g)^* = S^T S\, \rho'_{\boldsymbol{R}}(g)\, S^\dagger S^*\,, \tag{2.12}$$

and one can define the unitary matrix $U \coloneqq S^\dagger S^*$. Moreover, the field φ' is not real, but it fulfils the (generalised) reality condition[3]

$$\varphi' = S^\dagger \varphi = S^\dagger \varphi^* = S^\dagger S^* (\varphi')^* = U (\varphi')^*\,. \tag{2.13}$$

1 The matrix U is unitary. Contrary to that, one line of the unitary Clebsch–Gordan matrix $C_{ab,kjl}$ written down as a matrix in the indices a and b for fixed k, j, l has a wrong normalisation. This mismatch is encoded in α. In the example above, α is equal to $1/\sqrt{3}$.

2 In fact, that was already the case in the T′ example of the previous discussion.

3 This is, in a sense, an analogue of the Majorana condition for Dirac spinors.

Indeed, this is the only type of reality condition that can be imposed on fields in a pseudo-real representation. The canonical kinetic term of the real scalar field in the new basis turns into

$$\mathcal{L} \supset \frac{1}{2} (\partial_\mu \varphi')^T U^* (\partial^\mu \varphi') \tag{2.14}$$

and, since U^* is not necessarily positive definite, it might seem that the resulting propagator is unphysical. However, the new path integral measure is $\mathcal{D}\varphi' \sim \mathcal{D}(S^{-1}\varphi)$ and does not run over all real field values but over all values that satisfy the generalised reality condition (2.13). For all these values, the kinetic term is positive.

Although physically equivalent, a choice of basis which is not manifestly real is less suitable for performing explicit perturbative calculations since one cannot use the standard Feynman rules for real scalar fields. However, one can, for example, use the following procedure to carry out computations. One starts with a complex field with complex kinetic term and drops any reality condition. The reality condition is then imposed dynamically by a Lagrange multiplier. To this end, one extends the model by a complex auxiliary field z in the same representation as φ without any kinetic term and adds the terms

$$\mathcal{L} \supset z^\dagger (\varphi - U \varphi^*) + (\varphi^\dagger - \varphi^T U^\dagger) z + \xi |z|^2 \tag{2.15}$$

to the Lagrangian, where U is the same matrix as above. For $\xi \to 0$, the equations of motion of the auxiliary field z enforce the reality condition on φ. Thus, one can read off the Feynman rules from this Lagrangian and perform the loop calculations which, however, involve the field z on internal lines. After obtaining the result, one performs the limit $\xi \to 0$ to project out the contributions of φ that do not obey $\varphi = U \varphi^*$. Although it is thus possible to do computations in a not manifestly real basis, it is probably better to avoid this, if possible, and to work in a real basis, where one can use the usual Feynman rules.

A.3 Wigner's representation theorem

Quantum mechanical states are described by vectors in a projective Hilbert space PH, i.e. in the projective space obtained from a Hilbert space H where any two Hilbert space vectors that differ by a (non-zero) complex scalar multiple are identified. A symmetry can be defined as a bijective transformation acting on the states of the projective Hilbert space such that all transition probabilities between physically realisable states are preserved [178]. According to a famous theorem by Wigner [220], cf. also [165], all these operations on the projective Hilbert space PH can be elevated to operations on the Hilbert space H itself.[4] In fact, a symmetry is either represented on H by a linear and unitary operator $\boldsymbol{A}$,

$$\begin{aligned} \boldsymbol{A}\ (\lambda\ |v\rangle + \mu\ |w\rangle) &= \lambda\, \boldsymbol{A}\ |v\rangle + \mu\, \boldsymbol{A}\ |w\rangle\ , \\ \langle \boldsymbol{A}\, v \,|\, \boldsymbol{A}\, w\rangle &= \langle v \,|\, w\rangle\ , \end{aligned} \qquad \forall\, v, w \in H \text{ and } \lambda, \mu \in \mathbb{C}\,, \tag{3.1}$$

or by an anti-linear and unitary operator $\boldsymbol{B}$

$$\begin{aligned} \boldsymbol{B}\ (\lambda\ |v\rangle + \mu\ |w\rangle) &= \lambda^*\, \boldsymbol{B}\ |v\rangle + \mu^*\, \boldsymbol{B}\ |w\rangle\ , \\ \langle \boldsymbol{B}\, v \,|\, \boldsymbol{B}\, w\rangle &= \langle w \,|\, v\rangle\ , \end{aligned} \qquad \forall\, v, w \in H \text{ and } \lambda, \mu \in \mathbb{C}\,. \tag{3.2}$$

For anti-linear, unitary operators the terminology anti-unitary is also common.

4 Issues connected to superselection rules are ignored here, cf. [178].

A.4 Proofs concerning generalised CP transformations

In this appendix, the proofs concerning generalised CP transformations omitted in the main text are collected.

A.4.1 Class-inverting automorphisms of higher order

Let u be a class-inverting automorphism which is of order greater than two, i.e. which is not involutory. Moreover, assume that it squares to an inner automorphism,

$$\exists\, a \in G : u^2(g) = aga^{-1}\,, \qquad \forall\, g \in G\,. \tag{4.1}$$

In all checked examples, there is a second, involutory automorphism u' such that

$$\exists\, b \in G : u'(g) = bu(g)b^{-1}\,, \qquad \forall\, g \in G\,. \tag{4.2}$$

From the requirement that u' be involutory one obtains

$$u'^2(g) = bu(u'(g))b^{-1} = bu(bu(g)b^{-1})b^{-1} = bu(b)aga^{-1}u(b)^{-1}b^{-1} = g\,, \qquad \forall\, g \in G\,. \tag{4.3}$$

This is true if and only if

$$bu(b)a \in Z(G)\,. \tag{4.4}$$

Summarising, given a class-inverting automorphism u of order greater than two which fulfils (4.1), there is an equivalent involutory automorphism if and only if[5]

$$\exists\, b \in G : bu(b)a \in Z(G)\,. \tag{4.5}$$

For some sets of automorphisms, one can prove that such an element b can always be found.

As a first step, one can show using representation theory that $u(a) = az$ where z is in the centre of G. To this end, consider the action of u^2 on the matrix realisation of an irreducible representation $\boldsymbol{R}_i$,

$$\rho_i(u^2(g)) = \rho_i(a)\,\rho_i(g)\,\rho_i(a)^\dagger = U_i\,U_i^*\,\rho_i(g)\,U_i^T\,U_i^\dagger = V_i\,\rho_i(g)\,V_i^\dagger \tag{4.6}$$

with

$$V_i = U_i\,U_i^*\,. \tag{4.7}$$

By Schur's lemma

$$\rho_i(a) = \mathrm{e}^{-\mathrm{i}\,\alpha_i}\; V_i\,, \tag{4.8}$$

where α_i is some real phase.[6] Consider now

$$\rho_i(u(a)) = U_i\,\left(\mathrm{e}^{-\mathrm{i}\,\alpha_i}\; U_i\,U_i^*\right)^*\,U_i^\dagger = \mathrm{e}^{\mathrm{i}\;\alpha_i}\;U_i\,U_i^* = \mathrm{e}^{2\,\mathrm{i}\,\alpha_i}\;\rho_i(a)\,. \tag{4.9}$$

5 A similar but due to different assumptions more restrictive condition has been found in [188].

6 This also shows that the V_i are group elements up to a phase factor. This phase factor may result in an enlarged discrete symmetry. However, since it is diagonal for each irreducible representation, the discrete symmetry can only be enlarged to a direct product of G with an abelian factor.

Since u is an automorphism, its image must be a group element, i.e.

$$\exists\, b \in G : \rho_i(b) = \mathrm{e}^{2\,\mathrm{i}\,\alpha_i}\, \rho_i(a)\,. \tag{4.10}$$

This implies that

$$\rho_i(ab^{-1}) = \mathrm{e}^{-2\,\mathrm{i}\,\alpha_i}\, \mathbb{1} \tag{4.11}$$

represents an element z of G.[7] Since its matrix realisation commutes with all other elements of the group for each irreducible representation, the group element z is in the centre $Z(G)$. In conclusion,

$$u(a) = az\,, \tag{4.12}$$

i.e. a is a fixed-point of u up to an element in the centre of G.

One has now to distinguish the cases that the order of u is odd, ord $(u) = 2n + 1$, and that it is even, ord$(u) = 2n$.

Let first ord $(u) = 2n + 1$. Only ambivalent groups can have odd-order class-inverting automorphisms at all.[8] Then using (4.1) and (4.12)

$$u^{2n+1}(g) = g = u(a)^n u(g) u(a)^{-n} = a^n z^n u(g) a^{-n} z^{-n} = a^n u(g) a^{-n}\,, \qquad \forall\, g \in G\,, \tag{4.13}$$

i.e. the automorphism is inner. Thus, it is connected to the identity automorphism by the conjugation with $b = a^n$. Since the group is ambivalent, the identity automorphism is class-inverting and involutory.

Let now ord $(u) = 2n$, which, as explained, is always the case for non-ambivalent groups. Then a^n is in the centre $Z(G)$ of G. This can be directly seen from the defining equation for the order of u using equation (4.1),

$$u^{2n}(g) = g = a^n g a^{-n}\,, \qquad \forall\, g \in G \Rightarrow a^n \in Z(G)\,. \tag{4.14}$$

Let now $n = 2m+1$, i.e. ord $(u) = 4m+2$. One can then construct a solution b to equation (4.5) in the following way. Since a is a fixed-point of u up to an element z of the centre of G, according to (4.12), the choice $b = a^m$ solves equation (4.4) because

$$bu(b)a = a^m (az)^m a = a^{2m+1} z^m = a^n z^m \in Z(G)\,, \tag{4.15}$$

where it has been used that, as shown above, $a^n \in Z(G)$.

This argument also covers all non-abelian groups of odd order because the order of their elements is odd, i.e. ord $(a) = 2k + 1$ for some k. Then $b = a^k$ can be used to construct a class-inverting, involutory automorphism out of the higher-order one.

In conclusion, it was shown that any class-inverting automorphism that squares to an inner automorphism can be related by an inner automorphism to a class-inverting, involutory automorphism if one of the following is true: either the order of the group is odd or the order of the original automorphism is odd or the order of the original automorphism is $4m + 2$ for some natural number m. The only caveats are, hence, automorphisms of order $4m$.

Moreover, we have not been able to find a class-inverting automorphism that is not linked in the prescribed way to a class-inverting, involutory automorphism in any group up to order 300 using GAP; however, some groups of orders 128, 162, 192, 250, 256 and 288 could not be checked for computational reasons.

7 This also shows that G is maximally enlarged to $G \times \mathbb{Z}_2$.

8 For all other groups there would be at least one conjugacy class that is mapped to its inverse class by an odd power of the automorphism, i.e. an odd power cannot be the identity.

A.4.2 Class-inverting automorphisms that do not square to an inner automorphism

Let $v = u^2$, where v is not an inner automorphism of G.[9] Then

$$\rho_{\boldsymbol{R}_i}(v(g)) = V_i\, \rho_{\boldsymbol{R}_i}(g)\, V_i^{-1}\,, \qquad \forall\, g \in G\,, \forall\, i \tag{4.16}$$

but

$$\nexists\, a \in G:\ \forall\, i:\ \rho_{\boldsymbol{R}_i}(v(g)) = \rho_{\boldsymbol{R}_i}(a)\, \rho_{\boldsymbol{R}_i}(g)\, \rho_{\boldsymbol{R}_i}(a)^{-1}\,. \tag{4.17}$$

Thus, V_i cannot be written as

$$V_i = V_i'\, \rho_i(a) \tag{4.18}$$

for any a in G and with matrices V_i' which commute with the representation matrices of all group elements of G. Otherwise, one would obtain a contradiction with (4.17). Hence, the group $H = G \rtimes_v \mathbb{Z}_{\text{ord }(v)}$ obtained by promoting V_i to a symmetry is a non-trivial semi-direct product, i.e. it is not a direct product.

A.4.3 No class-inverting automorphism for odd-order non-abelian groups

Let us show, using the results obtained above, that non-abelian groups of odd order do not admit class-inverting automorphisms that square to inner automorphisms.[10] A remarkable implication of this is that non-abelian groups of odd order do not admit bases with real Clebsch–Gordan coefficients. The proof follows the lines of [187].

It is known that any class-inverting automorphism of an odd-order non-abelian group is fixed-point free [186]. This is true because the only real conjugacy class of such groups is the identity class. Thus, any involutory, class-inverting automorphism would be order two and fixed-point free. However, the existence of such an automorphism contradicts the assumption that the group is non-abelian. This can be seen as follows. Consider a group G and let τ be an order two, fixed-point free automorphism. Then the map

$$g \longmapsto g^{-1}\, \tau(g) \tag{4.19}$$

is injective because

$$g^{-1}\tau(g) = h^{-1}\tau(h) \qquad \Leftrightarrow \qquad hg^{-1} = \tau(hg^{-1})\,, \tag{4.20}$$

which is impossible as τ is fixed-point free. An injective map on a finite set is automatically bijective, and, hence, one can write every element $g \in G$ as $h^{-1}\tau(h)$ for some $h \in G$. This implies that the automorphism τ acts on group elements as inversion,

$$\tau(g) = \tau(h^{-1}\tau(h)) = \tau(h)^{-1}\, h = g^{-1}\,. \tag{4.21}$$

However, a group for which inversion is an automorphism is abelian,

$$gh = (h^{-1}g^{-1})^{-1} = \tau(h^{-1}g^{-1}) = \tau(h^{-1})\tau(g^{-1}) = hg\,, \qquad \forall\, g,h \in G\,, \tag{4.22}$$

9 Note that there are class-preserving automorphisms that are not inner automorphisms, e.g. for the group SG(32,43).

10 We cannot exclude the possibility that there are class-inverting automorphisms that square to non-inner automorphisms. However, there is no example up to group order 599 as we have checked explicitly using GAP.

which contradicts the assumption that the group is non-abelian.

Hence, there can be no involutory, class-inverting automorphism for non-abelian groups of odd order. This immediately implies that there is no basis with real Clebsch–Gordan coefficients for such groups.

This result can be extended in the following way. Let u be a class-inverting automorphism of order greater than two that squares to an inner automorphism,

$$\exists\, a \in G : u^2(g) = aga^{-1}\,, \qquad \forall\, g \in G\,. \tag{4.23}$$

Since the order of G is odd, there is a natural number m such that $a^{2m+1} = e$. Then, as shown in Section A.4.1, the automorphism

$$u'(g) = a^m u(g) a^{-m}\,, \qquad \forall\, g \in G \tag{4.24}$$

is class-inverting and involutory. However, this leads to a contradiction because a non-abelian group of odd order does not possess such an automorphism. Therefore, no higher-order class-inverting automorphism with the property (4.23) exists.

In summary, odd-order non-abelian groups do not have a basis with real Clebsch–Gordan coefficients and do not allow for consistent CP transformations in generic settings (with the possible caveat of automorphisms that square to non-inner automorphisms).

A.4.4 Class-inverting automorphisms of direct product groups

Since the conjugacy classes of a direct product group $G \times H$ are the Cartesian products of the classes of G and H, the product of two class-inverting automorphisms of G and H, respectively, is a class-inverting automorphism of the direct product group. If the automorphisms are both Bickerstaff–Damhus automorphisms, their Cartesian product is a Bickerstaff–Damhus automorphism of the direct product group because

$$\rho(u(g,h))^* = \rho(u(g,e))^*\, \rho(u(e,h))^* = \rho(g,e)\, \rho(e,h) = \rho(g,h)\,. \tag{4.25}$$

A.4.5 The extended twisted Frobenius–Schur indicator

Here we prove that the extended twisted Frobenius–Schur indicator (VII.6.6) can be used to check whether an automorphism τ of arbitrary order is class-inverting. Let $n := \mathrm{ord}\,(\tau)/2$ for even-order and $n := \mathrm{ord}\,(\tau)$ for odd-order automorphisms. Then (VII.6.6) can be written in component form as

$$\begin{aligned} \mathrm{FS}^n_\tau(\boldsymbol{R}_i) = \frac{(\dim \boldsymbol{R}_i)^{n-1}}{|G|^n} \sum_{g_1,\cdots,g_n \in G} & \left[\rho_{\boldsymbol{R}_i}(g)\right]_{a_1 b_1} \left[\rho_{\boldsymbol{R}_i}(\tau(g))\right]_{b_1 c_1}\, \delta_{c_1 a_2} \cdots \\ & \cdots \left[\rho_{\boldsymbol{R}_i}(g)\right]_{a_n b_n} \left[\rho_{\boldsymbol{R}_i}(\tau(g))\right]_{b_n c_n}\, \delta_{c_n a_1}\,. \end{aligned} \tag{4.26}$$

To this, one can apply the Schur orthogonality relations of Theorem 10, using the statement from Section VII.4.2 that the irreducible representations realised by $\rho_{\boldsymbol{R}_i}(g)$ and $\rho_{\boldsymbol{R}_i}(\tau(g))^*$ are equivalent for all i if and only if τ is class-inverting. Hence, if τ is not class-inverting, according to Theorem 10, the extended twisted Frobenius–Schur indicator vanishes for at least one irreducible representation.

Let now τ be class-inverting. Then the consistency equation (VII.4.24) has a solution, i.e. there is a unitary matrix U_i for each irreducible representation $\boldsymbol{R}_i$ such that

$$U_i\, \rho_{\boldsymbol{R}_i}(g)^*\, U_i^{-1} = \rho_{\boldsymbol{R}_i}(\tau(g))\,, \qquad \forall\, g \in G\,, \forall\, i\,. \tag{4.27}$$

Each factor of equation (4.26) can now be simplified to

$$\begin{aligned}
&\frac{1}{|G|}\sum_{g_k\in G}\left[\rho_{\boldsymbol{R}_i}(g_k)\right]_{a_kb_k}\left[\rho_{\boldsymbol{R}_i}(\tau(g_k))\right]_{b_kc_k} = \\
&\quad= \frac{1}{|G|}\sum_{g_k\in G}\left[\rho_{\boldsymbol{R}_i}(g_k)\right]_{a_kb_k}[U_i]_{b_kl}\left[\rho_{\boldsymbol{R}_i}(g_k)^*\right]_{lm}[U_i^{-1}]_{mc_k} \\
&\quad= \frac{1}{\dim \boldsymbol{R}_i}\,\delta_{a_kl}\,\delta_{b_km}\,[U_i]_{b_kl}\,[U_i^*]_{c_km} \\
&\quad= \frac{1}{\dim \boldsymbol{R}_i}\,[U_i^*\,U_i]_{c_ka_k}\,.
\end{aligned} \tag{4.28}$$

Hence, the extended twisted Frobenius–Schur indicator is

$$\begin{aligned}
\mathrm{FS}_\tau^n(\boldsymbol{R}_i) &= \frac{1}{\dim \boldsymbol{R}_i}\,\delta_{c_na_1}\,[U_i^*\,U_i]_{c_na_n}\cdots\delta_{c_2a_3}\,[U_i^*\,U_i]_{c_2a_2}\,\delta_{c_1a_2}\,[U_i^*\,U_i]_{c_1a_1} \\
&= \frac{1}{\dim \boldsymbol{R}_i}\,\mathrm{tr}\left[(U_i^*\,U_i)^n\right].
\end{aligned} \tag{4.29}$$

Since the trace is cyclic, the indicator is real. Moreover, inserting equation (VII.4.24) $2n$ times into itself,

$$\rho_{\boldsymbol{R}_i}(\tau^{2n}(g)) = (U_i\,U_i^*)^n\;\rho_{\boldsymbol{R}_i}(g)\;(U_i\,U_i^*)^{-n} = \rho_{\boldsymbol{R}_i}(g)\,,\qquad \forall\, g\in G\,,\forall\, i\,, \tag{4.30}$$

where in the last step the assumption on the order of τ was used. Hence, due to Schur's lemma, $(U_i\,U_i^*)^n$ is proportional to the unit matrix. As its trace is real, in fact, $(U_i\,U_i^*)^n = \pm\mathbb{1}$. This can be inserted back into (4.29) to show that the n-th extended twisted Frobenius–Schur indicator is ±1 for class-inverting automorphisms τ and zero for at least one irreducible representation for all other automorphisms.

A.5 Strong Gelfand pairs

A pair of (finite) group G and subgroup $H\subset G$ such that the decomposition of each irreducible representation of G into irreducible representations of H does not contain any irreducible representation of H more than once is called strong Gelfand pair [221].[11] This is the case if and only if the algebra of complex-valued functions f on the group G that are invariant under conjugation with H,[12] i.e.

$$f(hgh^{-1}) = f(g)\,,\qquad \forall\, g\in G \text{ and } \forall\, h\in H\,, \tag{5.1}$$

with respect to the multiplication

$$[f_1 * f_2](\tilde g) := \sum_{g\in G} f_1(\tilde g\, g) f_2(g^{-1}) \tag{5.2}$$

is commutative [221]. As shown in [214], this is the same as the criterion that the equivalence classes with respect to conjugation by H commute in G.

11 For information on normal Gelfand pairs see [222].

12 The set of all irreducible characters forms a basis of the $\mathbb{C}$ vector space of functions $G\to\mathbb{C}$ that are invariant on (G-)conjugacy classes.

A sufficient condition that G and H are a strong Gelfand pair is the existence of an anti-automorphism[13] τ such that

$$\forall\, g \in G\, \exists\, h \in H : \tau(g) = hgh^{-1}\,. \tag{5.3}$$

This can be seen using the definition of the algebra multiplication and the fact that $f(g) = f(\tau(g))$:

$$\begin{aligned}
[f_1 * f_2](\tilde{g}) &= \sum_{g\in G} f_1(\tilde{g}\,g) f_2(g^{-1}) \\
&= \sum_{g\in G} f_1(\tau(\tilde{g}\,g)) f_2(\tau(g^{-1})) \\
&= \sum_{h\in G} f_1(\tau(h)^{-1}) f_2(\tau(h\,\tilde{g})) \\
&= \sum_{h\in G} f_2(\tau(\tilde{g})\,\tau(h)) f_1(\tau(h)^{-1}) \\
&= [f_2 * f_1](\tau(\tilde{g})) \\
&= [f_2 * f_1](\tilde{g})\,.
\end{aligned} \tag{5.4}$$

One can alternatively use the criterion that the H conjugacy classes C_i^H in G have to commute, i.e. the criterion by Wigner [214], to show that a group–subgroup pair with such an anti-automorphism is a Strong Gelfand pair. For this let $\tilde{g} \in C_1^H\, C_2^H$. Then $g = \tau^{-1}(\tilde{g})$ is also in $C_1^H\, C_2^H$ and can, therefore, be written as a product $g_1 g_2$ with $g_i \in C_i^H$. Moreover, it holds that

$$\tilde{g} = \tau(g) = \tau(g_1 g_2) = \tau(g_2)\,\tau(g_1) \in C_2^H\, C_1^H\,. \tag{5.5}$$

Since this holds for all $\tilde{g} \in C_1^H\, C_2^H$ and the reversed argument also for all elements $\tilde{g} \in C_2^H\, C_1^H$, it follows that

$$C_1^H\, C_2^H = C_2^H\, C_1^H\,. \tag{5.6}$$

Note that anti-automorphisms can be constructed from the composition of automorphisms with group inversion, which is itself an anti-automorphism. One might thus be led to think that one could obtain an anti-automorphism fulfilling (5.3) from any class-inverting automorphism of G by composing it with group inversion. This is not the case. Even if the restriction of the automorphism to the subgroup H is class-inverting for H, its composition with inversion might not have the desired property. In fact, there might be an element $a \in G \setminus H$ such that $u(a) = ka^{-1}k^{-1}$ only for elements $k \in G \setminus H$. Indeed, A_5 has S_3 as a maximal subgroup and, because both are ambivalent groups, the identity automorphism is class-inverting for both of them. Nonetheless, the decomposition of A_5 representations to S_3 representations is not multiplicity free, namely the **5** of A_5 contains two **2**'s of S_3.

The existence of an anti-automorphism fulfilling (5.3) is thus a stronger requirement for a group–subgroup pair (G, H) than the existence of a class-inverting automorphism of G that restricts to a class-inverting automorphism of H.

13 An anti-automorphism is a bijective function on the group that fulfils $\tau(g_1 g_2) = \tau(g_2)\,\tau(g_1)$ for all $g_1, g_2 \in G$. Sometimes it is also demanded that τ is an involution, i.e. $\tau^2 = \mathrm{id}$; however, this is not needed for the proof.

A.6 Matrix decompositions and normal forms

A.6.1 Positive Hermitian matrices

A matrix A representing an endomorphism on V is called positive semi-definite if

$$\langle A\,v,\, v\rangle \geq 0\,, \qquad \forall\, v \in V\,, \tag{6.1}$$

and positive definite if $\geq$ can be replaced with $>$.

If A is positive semi-definite and Hermitian, there is a unique positive semi-definite matrix S such that [139]

$$A = S^\dagger\, S = S^2\,. \tag{6.2}$$

S is sometimes denoted by $A^{1/2}$.

A.6.2 Singular value decomposition

Any matrix[14] A has a unique polar decomposition [139]

$$A = V\,H\,. \tag{6.3}$$

where V is unitary and H the positive semi-definite Hermitian matrix

$$H = (A^\dagger\, A)^{1/2}\,. \tag{6.4}$$

H is unitarily diagonalised by a matrix U,

$$H = U\ \mathrm{diag}\,(\sigma_i)\ U^\dagger\,, \tag{6.5}$$

with eigenvalues σ_i which are the square roots of the eigenvalues of $A^\dagger\, A$. Hence, one obtains that for any matrix A there is a singular value decomposition

$$A = V\,U\ \mathrm{diag}\,(\sigma_i)\ U^\dagger =: V'\ \mathrm{diag}\,(\sigma_i)\ U^\dagger \tag{6.6}$$

with unitary V' and U. The values σ_i are called singular values of A. Even assuming that all singular values are distinct and fixing their order, V' and U are only defined up to multiplication with a diagonal phase matrix U^{ph},

$$V' \mapsto V'\,U^{\mathrm{ph}}\,, \tag{6.7a}$$

$$U \mapsto U\,U^{\mathrm{ph}}\,, \tag{6.7b}$$

because this phase change does not affect equation (6.6). For n degenerate singular values this ambiguity is extended to $\mathrm{U}(n)$ for the degenerate subspace.

14 In fact, one can extend this to bounded linear operators on a Hilbert space.

A.6.3 Takagi factorisation

Any complex symmetric matrix $A = A^T$ can be written using a unitary transformation U as [223]

$$A = U\,D\,U^T = U\ \mathrm{diag}\,(\sigma_1, \ldots, \sigma_n)\,U^T\,, \tag{6.8}$$

where the σ_i are the singular values of A (see Section A.6.2 and also [224]). That is, the entries of the diagonal matrix D are the non-negative square roots of the absolute values of the eigenvalues of A or, equivalently, the non-negative square roots of the eigenvalues of $A\,A^\dagger$. This so-called Takagi factorisation is a special case of the singular value decomposition described in Section A.6.2. It is the matrix decomposition used to obtain the mass eigenstates of a Majorana mass matrix. In the present text, it is also applied to symmetric CP transformation matrices U_{CP}.

A.6.4 Normal form of unitary matrices

Ecker, Grimus and Neufeld [24] showed that a general unitary matrix U can be written as the product

$$U = V^T \begin{pmatrix} O_1 & & & \\ & \ddots & & \\ & & O_l & \\ & & & \mathbb{1}_m \end{pmatrix} V\,, \tag{6.9}$$

with a unitary matrix V and where the O_i are two-dimensional orthogonal matrices,

$$O_i = \begin{pmatrix} \cos\theta_i & \sin\theta_i \\ -\sin\theta_i & \cos\theta_i \end{pmatrix}\,. \tag{6.10}$$

The angles θ_i are determined by the eigenvalues $\cos^2(\theta_i)$ and 1 of the Hermitian matrix

$$\frac{1}{4}\,(U + U^T)^\dagger\,(U + U^T) \tag{6.11}$$

or, alternatively, by the eigenvalues $\mathrm{e}^{\pm 2\,\mathrm{i}\,\theta_i}$ of $U\,U^*$.

B Kinetic corrections to tri-bi-maximal mixing

In this appendix, results are presented for kinetic corrections to the mixing angles of tri-bi-maximal mixing as defined in Table V.4. Only contributions from the left-handed doublets, i.e. from Kähler potentials of the form

$$K = L^\dagger \left(\mathbb{1} + x_L P_L\right) L + R^\dagger R \tag{0.1}$$

or equivalent kinetic terms, are shown, where P_L is replaced by one of the nine basis matrices P_i from equation (V.4.25).

Since $\theta_{13} = 0$ as initial condition, the initial CP phase δ_{CP} is not well defined. It is determined from the formulas by demanding that the change of δ_{CP} be analytical at $\theta_{13} = 0$ for each of the P_i individually, which yields $\delta = 0$ for $i = 1, \ldots, 6$ and $\delta = -\pi/2$ for $i = 7, 8, 9$. The neutrino masses m_{ν_i} are left unspecified. The hierarchy $m_\tau \gg m_\mu \gg m_e$ of the charged lepton masses is used to simplify the results. To first order in an expansion in the small mass ratios, the charged lepton masses completely drop out from the formulas.

The results are listed in the following:

- For $P_L = P_1$:

$$\Delta\theta_{12}^{(1)} = x_L \frac{1}{3\sqrt{2}} \frac{m_{\nu_1} + m_{\nu_2}}{m_{\nu_1} - m_{\nu_2}} , \tag{0.2a}$$

$$\Delta\theta_{13}^{(1)} = 0 , \tag{0.2b}$$

$$\Delta\theta_{23}^{(1)} = 0 . \tag{0.2c}$$

- For $P_L = P_2$:

$$\Delta\theta_{12}^{(2)} = x_L \frac{1}{3\sqrt{2}} \frac{2\,m_{\nu_1} - m_{\nu_2}}{m_{\nu_1} - m_{\nu_2}} , \tag{0.3a}$$

$$\Delta\theta_{13}^{(2)} = x_L \frac{1}{3\sqrt{2}} \frac{3\,m_{\nu_1} m_{\nu_2} - 2\,m_{\nu_1} m_{\nu_3} - m_{\nu_2} m_{\nu_3}}{(m_{\nu_1} - m_{\nu_3})\,(m_{\nu_2} - m_{\nu_3})} , \tag{0.3b}$$

$$\Delta\theta_{23}^{(2)} = x_L \frac{1}{3} \frac{m_{\nu_3}\,(m_{\nu_1} - m_{\nu_2})}{(m_{\nu_1} - m_{\nu_2})\,(m_{\nu_2} - m_{\nu_3})} . \tag{0.3c}$$

- For $P_L = P_3$:

$$\Delta\theta_{12}^{(3)} = -x_L \frac{1}{6\sqrt{2}} \frac{m_{\nu_1} + m_{\nu_2}}{m_{\nu_1} - m_{\nu_2}} , \tag{0.4a}$$

$$\Delta\theta_{13}^{(3)} = x_L \frac{1}{3\sqrt{2}} \frac{m_{\nu_3}(m_{\nu_1} - m_{\nu_2})}{(m_{\nu_1} - m_{\nu_3})(m_{\nu_2} - m_{\nu_3})} , \tag{0.4b}$$

$$\Delta\theta_{23}^{(3)} = x_L \frac{1}{12} \frac{m_{\nu_1}(3m_{\nu_2} + m_{\nu_3}) - m_{\nu_3}(m_{\nu_2} + 3m_{\nu_3})}{(m_{\nu_1} - m_{\nu_3})(m_{\nu_2} - m_{\nu_3})} . \tag{0.4c}$$

- For $P_L = P_4$:

$$\Delta\theta_{12}^{(4)} = x_L \frac{1}{3\sqrt{2}} \frac{2m_{\nu_1} - m_{\nu_2}}{m_{\nu_1} - m_{\nu_2}} , \tag{0.5a}$$

$$\Delta\theta_{13}^{(4)} = -x_L \frac{1}{3\sqrt{2}} \frac{3m_{\nu_1}m_{\nu_2} - 2m_{\nu_1}m_{\nu_3} - m_{\nu_2}m_{\nu_3}}{(m_{\nu_1} - m_{\nu_3})(m_{\nu_2} - m_{\nu_3})} , \tag{0.5b}$$

$$\Delta\theta_{23}^{(4)} = -x_L \frac{1}{3} \frac{m_{\nu_3}(m_{\nu_1} - m_{\nu_2})}{(m_{\nu_1} - m_{\nu_3})(m_{\nu_2} - m_{\nu_3})} . \tag{0.5c}$$

- For $P_L = P_5$:

$$\Delta\theta_{12}^{(5)} = -x_L \frac{1}{3\sqrt{2}} \frac{m_{\nu_1} + m_{\nu_2}}{m_{\nu_1} - m_{\nu_2}} , \tag{0.6a}$$

$$\Delta\theta_{13}^{(5)} = 0 , \tag{0.6b}$$

$$\Delta\theta_{23}^{(5)} = -x_L \frac{1}{2} . \tag{0.6c}$$

- For $P_L = P_6$:

$$\Delta\theta_{12}^{(6)} = -x_L \frac{1}{6\sqrt{2}} \frac{m_{\nu_1} + m_{\nu_2}}{m_{\nu_1} - m_{\nu_2}} , \tag{0.7a}$$

$$\Delta\theta_{13}^{(6)} = -x_L \frac{1}{3\sqrt{2}} \frac{m_{\nu_3}(m_{\nu_1} - m_{\nu_2})}{(m_{\nu_1} - m_{\nu_3})(m_{\nu_2} - m_{\nu_3})} , \tag{0.7b}$$

$$\Delta\theta_{23}^{(6)} = x_L \frac{1}{12} \frac{m_{\nu_1}(3m_{\nu_2} + m_{\nu_3}) - m_{\nu_3}(m_{\nu_2} + 3m_{\nu_3})}{(m_{\nu_1} - m_{\nu_3})(m_{\nu_3} - m_{\nu_2})} . \tag{0.7c}$$

- For $P_L = P_7$:

$$\Delta\theta_{12}^{(7)} = 0 , \tag{0.8a}$$

$$\Delta\theta_{13}^{(7)} = -x_L \frac{1}{3\sqrt{2}} \frac{3m_{\nu_1}m_{\nu_2} + 2m_{\nu_1}m_{\nu_3} + m_{\nu_2}m_{\nu_3}}{(m_{\nu_1} + m_{\nu_3})(m_{\nu_2} + m_{\nu_3})} , \tag{0.8b}$$

$$\Delta\theta_{23}^{(7)} = 0 . \tag{0.8c}$$

- For $P_L = P_8$:

$$\Delta\theta_{12}^{(8)} = 0 , \tag{0.9a}$$

$$\Delta\theta_{13}^{(8)} = x_L \frac{1}{3\sqrt{2}} \frac{3m_{\nu_1}m_{\nu_2} + 2m_{\nu_1}m_{\nu_3} + m_{\nu_2}m_{\nu_3}}{(m_{\nu_1} + m_{\nu_3})(m_{\nu_2} + m_{\nu_3})} , \tag{0.9b}$$

$$\Delta\theta_{23}^{(8)} = 0 . \tag{0.9c}$$

- For $P_L = P_9$:

$$\Delta\theta_{12}^{(9)} = 0 , \tag{0.10a}$$

$$\Delta\theta_{13}^{(9)} = -x_L \frac{\sqrt{2}}{3} \frac{m_{\nu_3}(m_{\nu_1} - m_{\nu_2})}{(m_{\nu_1} + m_{\nu_3})(m_{\nu_2} + m_{\nu_3})} , \tag{0.10b}$$

$$\Delta\theta_{23}^{(9)} = 0 . \tag{0.10c}$$

C GAP codes

In the following, some GAP [20] codes used for the computations concerning class-inverting automorphisms are presented.

The function `isClassinverting` can be used to compute whether a given automorphism `aut` of a group G is class-inverting (return value `true`) or not (return value `false`). The inputs are the automorphism `aut`, a list `cclass` of conjugacy classes of G and a list `repcclass` with representatives for these classes. The result is obtained by comparing the conjugacy class that each element of `repcclass` is mapped to with the conjugacy class of its inverse.

```
isClassinverting:=function(aut,cclass,repcclass)
local j;
for j in repcclass do
  if PositionProperty(cclass,x->j^-1 in x)
      <>PositionProperty(cclass,x->(j^aut) in x) then
    return false;
  fi;
od;
return true;
end;
```

The following function computes the twisted Frobenius–Schur indicators (VII.6.1) with respect to the automorphism `aut` for all irreducible representations of a group `G`.

```
twistedFS:=function(G,aut)
local elG,tbl,irr,fsList;
elG:=Elements(G);
tbl:=CharacterTable(G);
irr:=Irr(tbl);
fsList:=List(elG,x->x*x^aut);
return List(irr,y->Sum(fsList,x->x^y))/Size(G);
end;
```

The next function computes the n-th order extended twisted Frobenius–Schur indicators (VII.6.6) for all irreducible representations of a group `G` with respect to the automorphism u provided as `aut`, where $n := \operatorname{ord} u/2$ for even $\operatorname{ord} u$ and $n = \operatorname{ord} u$ for odd $\operatorname{ord} u$.

```
twistedFSn:=function(G,aut)
```

```
local ord,n,elG,tbl,irr,elGaut,fsList,i;
ord:=Order(aut);
if ord=0 mod 2 then
  n:=ord/2;
else
  n:=ord;
fi;
elG:=Elements(G);
tbl:=CharacterTable(G);
irr:=Irr(tbl);
elGaut:=List(elG,x->x*x^aut);
fsList:=ShallowCopy(elGaut);
for i in [1..n-1] do
  fsList:=List(fsList,x->List(elGaut,y->x*y));
  fsList:=Flat(fsList);
od;
return List(irr,y->Sum(fsList,x->x^y)*y[1]^(n-1))/Size(G)^n;
end;
```

The last function presented here computes the inequivalent Bickerstaff–Damhus and class-inverting automorphisms of a group `G`. To this end, it generates the automorphism group of `G` and its coset decomposition with respect to the inner automorphism group. Then it loops over these classes, checking for each class whether its automorphisms are class-inverting. If this is not the case, the loop continuous. If the class consists of class-inverting automorphisms, for all of them the twisted Frobenius–Schur indicators are computed to check whether any of them is a Bickerstaff–Damhus automorphism. If a Bickerstaff–Damhus automorphism is found, a representative of the class is returned as part of the first list of the output. If no Bickerstaff–Damhus automorphism is found, i.e. the automorphisms of the class are all only class-inverting, a representative of the class is returned as part of the second list of the output. Moreover, for each case it is checked whether the automorphisms are inner automorphisms.

```
checkForCIAutomorphismsOutG:=function(G)
local i,j,autG,ordG,elG,tbl,chi,cclass,repcclass,innG,
    eloutGList,res,resTemp,aut,ci,maclist,fslists;
autG:=AutomorphismGroup(G);
ordG:=Size(G);
elG:=Elements(G);
tbl:= CharacterTable(G);
chi:=Irr(tbl);
cclass:=ConjugacyClasses(tbl);
repcclass:=List(cclass,x->Representative(x));
innG:=InnerAutomorphismsAutomorphismGroup(autG);
eloutGList:=CosetDecomposition(autG,innG);
res:=[[],[]];
for i in [1..Length(eloutGList)] do
  resTemp:=[];
  aut:=eloutGList[i][1];
  ci:=isClassinverting(aut,cclass,repcclass);
```

```
  if ci then
    for j in [1..Length(eloutGList[i])] do
      aut:=eloutGList[i][j];
      maclist:=List(elG,x->x*x^aut);
      fslists:=List(chi,y->Sum(maclist,x->x^y))/ordG;
      if ForAll(fslists,x->x=1) then
        Add(resTemp,[i,1]);
        break;
      else
        Add(resTemp,[i,2]);
      fi;
    od;
    if ForAny(resTemp,x->x[2]=1) then
      Add(res[1],[eloutGList[i][1],IsInnerAutomorphism(aut)]);
    elif ForAny(resTemp,x->x[2]=2) then
      Add(res[2],[eloutGList[i][1],IsInnerAutomorphism(aut)]);
    fi;
  fi;
od;
Print(res[1]," are Bickerstaff-Damhus automorphisms.\n");
Print(res[2]," are class-inverting automorphisms.\n");
return res;
end;
```

D CP transformations for small groups

The following table lists all groups of order 100 and smaller which are non-abelian and which are not direct product groups with their numbers of possible CP transformations.[1]

The first two columns of the table show the ID of the group with respect to the SmallGroups library of GAP [20] and the structure description of the group in GAP notation, respectively.

The third column contains the number of inequivalent Bickerstaff–Damhus automorphisms and the last column the number of inequivalent class-inverting automorphisms that are not Bickerstaff–Damhus automorphisms. Automorphisms are inequivalent if they are not in the same equivalence class of the outer automorphism group. A star is attached to the numbers if an inner automorphism is a Bickerstaff–Damhus automorphism or just class-inverting, respectively.

ID	Group structure	BDA	ci
[6, 1]	S3	1*	0
[8, 3]	D8	1*	0
[8, 4]	Q8	1*	0
[10, 1]	D10	1*	0
[12, 1]	C3 : C4	1	0
[12, 3]	A4	1	0
[14, 1]	D14	1*	0
[16, 3]	(C4 x C2) : C2	1	0
[16, 4]	C4 : C4	1	0
[16, 6]	C8 : C2	1	0
[16, 7]	D16	1*	0
[16, 8]	QD16	1	0
[16, 9]	Q16	1*	0
[16, 13]	(C4 x C2) : C2	1	0
[18, 1]	D18	1*	0
[18, 4]	(C3 x C3) : C2	1*	0
[20, 1]	C5 : C4	1	0
[20, 3]	C5 : C4	0	0
[21, 1]	C7 : C3	0	0
[22, 1]	D22	1*	0
[24, 1]	C3 : C8	1	0
[24, 3]	SL(2,3)	1	0
[24, 4]	C3 : Q8	1*	0
[24, 6]	D24	1*	0
[24, 8]	(C6 x C2) : C2	1	0
[24, 12]	S4	1*	0
[26, 1]	D26	1*	0
[27, 3]	(C3 x C3) : C3	0	0

1 For direct product groups, the automorphisms of their factors can just be combined, see Section A.4.4. Note that there might be additional automorphisms of the direct product group that cannot be constructed this way.

ID	Group structure	BDA	ci
[27, 4]	C9 : C3	0	0
[28, 1]	C7 : C4	1	0
[30, 3]	D30	1*	0
[32, 2]	(C4 x C2) : C4	1	0
[32, 4]	C8 : C4	1	0
[32, 5]	(C8 x C2) : C2	1	0
[32, 6]	((C4 x C2) : C2) : C2	1	0
[32, 7]	(C8 : C2) : C2	1	0
[32, 8]	C2 . ((C4 x C2) : C2) = (C2 x C2) . (C4 x C2)	1	0
[32, 9]	(C8 x C2) : C2	1	0
[32, 10]	Q8 : C4	1	0
[32, 11]	(C4 x C4) : C2	1	0
[32, 12]	C4 : C8	1	0
[32, 13]	C8 : C4	1	0
[32, 14]	C8 : C4	1	0
[32, 15]	C4 . D8 = C4 . (C4 x C2)	1	0
[32, 17]	C16 : C2	1	0
[32, 18]	D32	1*	0
[32, 19]	QD32	1	0
[32, 20]	Q32	1*	0
[32, 24]	(C4 x C4) : C2	1	0
[32, 27]	(C2 x C2 x C2 x C2) : C2	1*	0
[32, 28]	(C4 x C2 x C2) : C2	1	0
[32, 29]	(C2 x Q8) : C2	1	0
[32, 30]	(C4 x C2 x C2) : C2	1	0
[32, 31]	(C4 x C4) : C2	1	0
[32, 32]	(C2 x C2) . (C2 x C2 x C2)	1	0
[32, 33]	(C4 x C4) : C2	1	0
[32, 34]	(C4 x C4) : C2	1*	0
[32, 35]	C4 : Q8	1*	0
[32, 38]	(C8 x C2) : C2	1	0
[32, 42]	(C8 x C2) : C2	1	0
[32, 43]	(C2 x D8) : C2	2*	0
[32, 44]	(C2 x Q8) : C2	2*	0
[32, 49]	(C2 x D8) : C2	1*	0
[32, 50]	(C2 x Q8) : C2	1*	0
[34, 1]	D34	1*	0
[36, 1]	C9 : C4	1	0
[36, 3]	(C2 x C2) : C9	1	0
[36, 7]	(C3 x C3) : C4	1	0
[36, 9]	(C3 x C3) : C4	1	0
[38, 1]	D38	1*	0
[39, 1]	C13 : C3	0	0
[40, 1]	C5 : C8	1	0
[40, 3]	C5 : C8	0	0
[40, 4]	C5 : Q8	1*	0
[40, 6]	D40	1*	0
[40, 8]	(C10 x C2) : C2	1	0
[42, 1]	(C7 : C3) : C2	0	0
[42, 5]	D42	1*	0
[44, 1]	C11 : C4	1	0
[46, 1]	D46	1*	0
[48, 1]	C3 : C16	1	0
[48, 3]	(C4 x C4) : C3	0	0
[48, 5]	C24 : C2	1	0
[48, 6]	C24 : C2	1	0
[48, 7]	D48	1*	0
[48, 8]	C3 : Q16	1*	0
[48, 10]	(C3 : C8) : C2	1	0
[48, 12]	(C3 : C4) : C4	1	0
[48, 13]	C12 : C4	1	0
[48, 14]	(C12 x C2) : C2	1	0
[48, 15]	(C3 x D8) : C2	1	0
[48, 16]	(C3 : C8) : C2	1	0
[48, 17]	(C3 x Q8) : C2	1	0
[48, 18]	C3 : Q16	1	0

ID	Group structure	BDA	ci
[48, 19]	(C2 x (C3 : C4)) : C2	1	0
[48, 28]	C2 . S4 = SL(2,3) . C2	1*	0
[48, 29]	GL(2,3)	1	0
[48, 30]	A4 : C4	1	0
[48, 33]	SL(2,3) : C2	1	0
[48, 37]	(C12 x C2) : C2	1	0
[48, 39]	(C2 x (C3 : C4)) : C2	1	0
[48, 41]	(C4 x S3) : C2	1	0
[48, 50]	(C2 x C2 x C2 x C2) : C3	0	0
[50, 1]	D50	1*	0
[50, 4]	(C5 x C5) : C2	1*	0
[52, 1]	C13 : C4	1	0
[52, 3]	C13 : C4	0	0
[54, 1]	D54	1*	0
[54, 5]	((C3 x C3) : C3) : C2	1	0
[54, 6]	(C9 : C3) : C2	0	0
[54, 7]	(C9 x C3) : C2	1*	0
[54, 8]	((C3 x C3) : C3) : C2	0	0
[54, 14]	(C3 x C3 x C3) : C2	1*	0
[55, 1]	C11 : C5	0	0
[56, 1]	C7 : C8	1	0
[56, 3]	C7 : Q8	1*	0
[56, 5]	D56	1*	0
[56, 7]	(C14 x C2) : C2	1	0
[56, 11]	(C2 x C2 x C2) : C7	0	0
[57, 1]	C19 : C3	0	0
[58, 1]	D58	1*	0
[60, 3]	C15 : C4	1	0
[60, 5]	A5	1*	0
[60, 7]	C15 : C4	0	0
[62, 1]	D62	1*	0
[63, 1]	C7 : C9	0	0
[64, 3]	C8 : C8	1	0
[64, 4]	((C8 x C2) : C2) : C2	1	0
[64, 5]	(C4 x C2) : C8	1	0
[64, 6]	(C8 x C4) : C2	1	0
[64, 7]	Q8 : C8	1	0
[64, 8]	((C8 x C2) : C2) : C2	1	0
[64, 9]	(C2 x Q8) : C4	1	0
[64, 10]	(C8 : C4) : C2	1	0
[64, 11]	(C2 x C2) . ((C4 x C2) : C2) = (C4 x C2) . (C4 x C2)	1	0
[64, 12]	(C4 : C8) : C2	1	0
[64, 13]	(C2 x C2) . ((C4 x C2) : C2) = (C4 x C2) . (C4 x C2)	1	0
[64, 14]	(C2 x C2) . ((C4 x C2) : C2) = (C4 x C2) . (C4 x C2)	1	0
[64, 15]	C8 : C8	1	0
[64, 16]	C8 : C8	1	0
[64, 17]	(C8 x C2) : C4	1	0
[64, 18]	(C8 x C2) : C4	0	0
[64, 19]	C4 . (C4 x C4)	0	0
[64, 20]	(C4 x C4) : C4	1	0
[64, 21]	(C8 x C2) : C4	1	0
[64, 22]	(C4 x C2) . D8 = C4 . (C4 x C4)	1	0
[64, 23]	(C4 x C2 x C2) : C4	1	0
[64, 24]	(C8 : C2) : C4	1	0
[64, 25]	(C8 x C2) : C4	1	0
[64, 27]	C16 : C4	1	0
[64, 28]	C16 : C4	0	0
[64, 29]	(C16 x C2) : C2	1	0
[64, 30]	(C16 : C2) : C2	1	0
[64, 31]	(C16 x C2) : C2	1	0
[64, 32]	((C8 : C2) : C2) : C2	1	0
[64, 33]	(C4 x C2 x C2) : C4	1	0
[64, 34]	(((C4 x C2) : C2) : C2) : C2	1	0
[64, 35]	(C4 x C4) : C4	1	0
[64, 36]	(C2 . ((C4 x C2) : C2) = (C2 x C2) . (C4 x C2)) : C2	1	0
[64, 37]	C2 . (((C4 x C2) : C2) : C2) = (C4 x C2) . (C4 x C2)	1	0

ID	Group structure	BDA	ci
[64, 38]	(C16 x C2) : C2	1	0
[64, 39]	Q16 : C4	1	0
[64, 40]	(C16 x C2) : C2	1	0
[64, 41]	(C16 : C2) : C2	1	0
[64, 42]	(C16 : C2) : C2	1	0
[64, 43]	C2 . ((C8 x C2) : C2) = C8 . (C4 x C2)	1	0
[64, 44]	C4 : C16	1	0
[64, 45]	C8 . D8 = C4 . (C8 x C2)	1	0
[64, 46]	C16 : C4	0	0
[64, 47]	C16 : C4	1	0
[64, 48]	C16 : C4	1	0
[64, 49]	C4 . D16 = C8 . (C4 x C2)	1	0
[64, 51]	C32 : C2	1	0
[64, 52]	D64	1*	0
[64, 53]	QD64	1	0
[64, 54]	Q64	1*	0
[64, 57]	(C4 x C4) : C4	1	0
[64, 60]	(C2 x ((C4 x C2) : C2)) : C2	1	0
[64, 61]	(C2 x (C4 : C4)) : C2	1	0
[64, 62]	((C4 x C2) : C4) : C2	1	0
[64, 63]	(C4 x C4) : C4	1	0
[64, 64]	(C4 x C4) : C4	1	0
[64, 65]	(C4 x C4) : C4	1	0
[64, 66]	(C2 x (C4 : C4)) : C2	1	0
[64, 67]	(C4 x C2 x C2 x C2) : C2	1	0
[64, 68]	(C4 : C4) : C4	1	0
[64, 69]	(C4 x C4 x C2) : C2	1	0
[64, 70]	(C4 : C4) : C4	1	0
[64, 71]	(C4 x C4 x C2) : C2	1	0
[64, 72]	(C2 x Q8) : C4	1	0
[64, 73]	(C2 x C2 x D8) : C2	0	0
[64, 74]	(C2 x C2 x Q8) : C2	0	0
[64, 75]	(C2 x ((C4 x C2) : C2)) : C2	0	0
[64, 76]	(C4 x C2) : Q8	0	0
[64, 77]	(C2 x (C4 : C4)) : C2	0	0
[64, 78]	(C2 x (C4 : C4)) : C2	0	0
[64, 79]	(C2 x C2 x C2) . (C2 x C2 x C2)	0	0
[64, 80]	(C2 x (C4 : C4)) : C2	0	0
[64, 81]	(C2 x C2 x C2) . (C2 x C2 x C2)	0	0
[64, 82]	(C2 x C2 x C2) . (C2 x C2 x C2)	0	0
[64, 86]	(C8 x C4) : C2	1	0
[64, 88]	(C2 x (C8 : C2)) : C2	1	0
[64, 89]	(C8 x C2 x C2) : C2	1	0
[64, 91]	(((C4 x C2) : C2) : C2) : C2	1	0
[64, 94]	(C2 x (C8 : C2)) : C2	1	0
[64, 97]	(C8 x C2 x C2) : C2	1	0
[64, 98]	(C2 x (C8 : C2)) : C2	2	0
[64, 99]	(C2 x (C8 : C2)) : C2	2	0
[64, 100]	(Q8 : C4) : C2	2	0
[64, 102]	(C2 x (C8 : C2)) : C2	2	0
[64, 104]	(C4 : C8) : C2	1	0
[64, 105]	(C4 : C8) : C2	1	0
[64, 108]	(C8 : C4) : C2	1	0
[64, 109]	(C8 : C4) : C2	2	0
[64, 111]	(C4 . D8 = C4 . (C4 x C2)) : C2	2	0
[64, 112]	(C8 x C4) : C2	1	0
[64, 113]	(C4 : C8) : C2	1	0
[64, 114]	(C8 x C4) : C2	1	0
[64, 116]	(C8 x C2 x C2) : C2	1	0
[64, 117]	(C8 x C4) : C2	1	0
[64, 121]	(C4 x Q8) : C2	2	0
[64, 122]	Q16 : C4	2	0
[64, 123]	(C4 x D8) : C2	2	0
[64, 124]	(C8 x C4) : C2	1	0
[64, 125]	((C4 x C4) : C2) : C2	2	0
[64, 127]	C8 : Q8	1	0

ID	Group structure	BDA	ci
[64, 128]	(C2 x C2 x D8) : C2	1*	0
[64, 129]	(C2 x C2 x Q8) : C2	1	0
[64, 130]	(C2 x D16) : C2	1	0
[64, 131]	(C2 x QD16) : C2	1	0
[64, 132]	(C2 x Q16) : C2	1*	0
[64, 133]	(C2 x Q16) : C2	1	0
[64, 134]	((C4 x C4) : C2) : C2	1*	0
[64, 135]	((C4 x C4) : C2) : C2	1	0
[64, 136]	((C4 x C4) : C2) : C2	1	0
[64, 137]	((C4 x C4) : C2) : C2	1*	0
[64, 138]	(((C4 x C2) : C2) : C2) : C2	1*	0
[64, 139]	(((C4 x C2) : C2) : C2) : C2	1	0
[64, 140]	(C4 x D8) : C2	1	0
[64, 141]	(C2 x QD16) : C2	1	0
[64, 142]	(Q8 : C4) : C2	1	0
[64, 143]	C4 : Q16	1	0
[64, 144]	(C4 x D8) : C2	1	0
[64, 145]	(C2 x Q16) : C2	1	0
[64, 146]	(C8 x C2 x C2) : C2	1	0
[64, 147]	(C8 x C2 x C2) : C2	1	0
[64, 148]	(C2 x Q16) : C2	1	0
[64, 149]	(C2 x (C8 : C2)) : C2	4	0
[64, 150]	(C2 x (C8 : C2)) : C2	4	0
[64, 151]	(C2 x Q16) : C2	4	0
[64, 152]	(C2 x QD16) : C2	1	0
[64, 153]	(C2 x D16) : C2	1	0
[64, 154]	(C2 x Q16) : C2	1	0
[64, 155]	(C8 : C4) : C2	1	0
[64, 156]	Q8 : Q8	1	0
[64, 157]	(C8 : C4) : C2	1	0
[64, 158]	Q8 : Q8	1	0
[64, 159]	(C8 : C4) : C2	1	0
[64, 160]	(C2 x C2) . (C2 x D8) = (C4 x C2) . (C2 x C2 x C2)	1	0
[64, 161]	(C2 x (C4 : C4)) : C2	1	0
[64, 162]	(C2 x (C4 : C4)) : C2	1	0
[64, 163]	((C8 x C2) : C2) : C2	1	0
[64, 164]	(Q8 : C4) : C2	1	0
[64, 165]	(Q8 : C4) : C2	1	0
[64, 166]	(C8 : C4) : C2	1	0
[64, 167]	(C8 x C4) : C2	1	0
[64, 168]	(C2 x C2) . (C2 x D8) = (C4 x C2) . (C2 x C2 x C2)	1	0
[64, 169]	(C8 x C4) : C2	1	0
[64, 170]	(Q8 : C4) : C2	4	0
[64, 171]	((C8 x C2) : C2) : C2	4	0
[64, 172]	(C2 x C2) . (C2 x D8) = (C4 x C2) . (C2 x C2 x C2)	4	0
[64, 173]	(C8 x C4) : C2	1	0
[64, 174]	(C8 x C4) : C2	1*	0
[64, 175]	C4 : Q16	1*	0
[64, 176]	(C8 x C4) : C2	1	0
[64, 177]	(C2 x D16) : C2	4*	0
[64, 178]	(C2 x Q16) : C2	4*	0
[64, 179]	C8 : Q8	1	0
[64, 180]	(C2 x C2) . (C2 x D8) = (C4 x C2) . (C2 x C2 x C2)	1	0
[64, 181]	C8 : Q8	1*	0
[64, 182]	C8 : Q8	4*	0
[64, 185]	(C16 x C2) : C2	1	0
[64, 189]	(C16 x C2) : C2	1	0
[64, 190]	(C2 x D16) : C2	2*	0
[64, 191]	(C2 x Q16) : C2	2*	0
[64, 199]	(C4 x D8) : C2	1	0
[64, 200]	(C4 x Q8) : C2	1	0
[64, 201]	(C4 x Q8) : C2	1	0
[64, 206]	(C4 x C2 x C2 x C2) : C2	1	0
[64, 210]	(C4 x C4 x C2) : C2	1	0
[64, 213]	(C4 x C4 x C2) : C2	1	0
[64, 214]	(C4 x Q8) : C2	1	0

ID	Group structure	BDA	ci
[64, 215]	(C2 x C2 x D8) : C2	3*	1
[64, 216]	(C2 x C2 x D8) : C2	3*	1
[64, 217]	(C2 x C2 x Q8) : C2	3*	1
[64, 218]	(C2 x ((C4 x C2) : C2)) : C2	3	1*
[64, 219]	(C4 x D8) : C2	3	1
[64, 220]	(C4 x D8) : C2	3	1
[64, 221]	(C4 x D8) : C2	3	1
[64, 222]	(C4 x Q8) : C2	3	1
[64, 223]	(C4 x Q8) : C2	3	1
[64, 224]	((C2 x Q8) : C2) : C2	3	1*
[64, 225]	(C4 : Q8) : C2	3*	1
[64, 227]	(C2 x C2 x D8) : C2	1	0
[64, 228]	(C4 x D8) : C2	1	0
[64, 229]	(C2 x C2 x Q8) : C2	1	0
[64, 231]	(C4 x D8) : C2	1	0
[64, 232]	(C4 x D8) : C2	1	0
[64, 233]	(C4 x Q8) : C2	1	0
[64, 234]	(C4 x D8) : C2	1	0
[64, 235]	(C4 x Q8) : C2	1	0
[64, 236]	(C4 x D8) : C2	1	0
[64, 237]	(C4 x Q8) : C2	1	0
[64, 238]	Q8 : Q8	1	0
[64, 240]	(C4 x D8) : C2	1	0
[64, 241]	((C4 x C2 x C2) : C2) : C2	10*	6
[64, 242]	((C4 x C4) : C2) : C2	10*	6
[64, 243]	((C2 x C2) . (C2 x C2 x C2)) : C2	10	6*
[64, 244]	((C4 x C4) : C2) : C2	10*	6
[64, 245]	(C2 x C2) . (C2 x C2 x C2 x C2)	10	6*
[64, 249]	(C2 x (C8 : C2)) : C2	1	0
[64, 256]	(C2 x (C8 : C2)) : C2	2	0
[64, 257]	(C2 x D16) : C2	1*	0
[64, 258]	(C2 x QD16) : C2	1	0
[64, 259]	(C2 x Q16) : C2	1*	0
[64, 266]	(C2 x ((C4 x C2) : C2)) : C2	1	0
[66, 3]	D66	1*	0
[68, 1]	C17 : C4	1	0
[68, 3]	C17 : C4	0	0
[70, 3]	D70	1*	0
[72, 1]	C9 : C8	1	0
[72, 3]	Q8 : C9	1	0
[72, 4]	C9 : Q8	1*	0
[72, 6]	D72	1*	0
[72, 8]	(C18 x C2) : C2	1	0
[72, 13]	(C3 x C3) : C8	1	0
[72, 15]	((C2 x C2) : C9) : C2	1*	0
[72, 19]	(C3 x C3) : C8	1	0
[72, 21]	(C3 x (C3 : C4)) : C2	1	0
[72, 22]	(C6 x S3) : C2	1	0
[72, 23]	(C6 x S3) : C2	1	0
[72, 24]	(C3 x C3) : Q8	1*	0
[72, 31]	(C3 x C3) : Q8	1*	0
[72, 33]	(C12 x C3) : C2	1*	0
[72, 35]	(C6 x C6) : C2	1	0
[72, 39]	(C3 x C3) : C8	0	0
[72, 40]	(S3 x S3) : C2	1*	0
[72, 41]	(C3 x C3) : Q8	0	1*
[72, 43]	(C3 x A4) : C2	1*	0
[74, 1]	D74	1*	0
[75, 2]	(C5 x C5) : C3	0	0
[76, 1]	C19 : C4	1	0
[78, 1]	(C13 : C3) : C2	0	0
[78, 5]	D78	1*	0
[80, 1]	C5 : C16	1	0
[80, 3]	C5 : C16	0	0
[80, 5]	C40 : C2	1	0
[80, 6]	C40 : C2	1	0

ID	Group structure	BDA	ci
[80, 7]	D80	1*	0
[80, 8]	C5 : Q16	1*	0
[80, 10]	(C5 : C8) : C2	1	0
[80, 12]	(C5 : C4) : C4	1	0
[80, 13]	C20 : C4	1	0
[80, 14]	(C20 x C2) : C2	1	0
[80, 15]	(C5 x D8) : C2	1	0
[80, 16]	(C5 : C8) : C2	1	0
[80, 17]	(C5 x Q8) : C2	1	0
[80, 18]	C5 : Q16	1	0
[80, 19]	(C2 x (C5 : C4)) : C2	1	0
[80, 28]	(C5 : C8) : C2	0	0
[80, 29]	(C5 : C8) : C2	0	0
[80, 31]	C20 : C4	0	0
[80, 33]	(C5 : C8) : C2	0	0
[80, 34]	(C2 x (C5 : C4)) : C2	0	0
[80, 38]	(C20 x C2) : C2	1	0
[80, 40]	(C2 x (C5 : C4)) : C2	1	0
[80, 42]	(C4 x D10) : C2	1	0
[80, 49]	(C2 x C2 x C2 x C2) : C5	1	0
[81, 3]	(C9 x C3) : C3	0	0
[81, 4]	C9 : C9	0	0
[81, 6]	C27 : C3	0	0
[81, 7]	(C3 x C3 x C3) : C3	0	0
[81, 8]	(C9 x C3) : C3	0	0
[81, 9]	(C9 x C3) : C3	0	0
[81, 10]	C3 . ((C3 x C3) : C3) = (C3 x C3) . (C3 x C3)	0	0
[81, 14]	(C9 x C3) : C3	0	0
[82, 1]	D82	1*	0
[84, 1]	(C7 : C4) : C3	0	0
[84, 5]	C21 : C4	1	0
[84, 11]	(C14 x C2) : C3	0	0
[86, 1]	D86	1*	0
[88, 1]	C11 : C8	1	0
[88, 3]	C11 : Q8	1*	0
[88, 5]	D88	1*	0
[88, 7]	(C22 x C2) : C2	1	0
[90, 3]	D90	1*	0
[90, 9]	(C15 x C3) : C2	1*	0
[92, 1]	C23 : C4	1	0
[93, 1]	C31 : C3	0	0
[94, 1]	D94	1*	0
[96, 1]	C3 : C32	1	0
[96, 3]	((C4 x C2) : C4) : C3	0	0
[96, 5]	C48 : C2	1	0
[96, 6]	D96	1*	0
[96, 7]	C48 : C2	1	0
[96, 8]	C3 : Q32	1*	0
[96, 10]	(C3 : C8) : C4	1	0
[96, 11]	C12 : C8	1	0
[96, 12]	(C12 x C4) : C2	1	0
[96, 13]	(C3 x ((C4 x C2) : C2)) : C2	1	0
[96, 14]	(C3 : C8) : C4	1	0
[96, 15]	(C3 : C8) : C4	1	0
[96, 16]	(C2 x (C3 : C8)) : C2	1	0
[96, 17]	(C3 : Q8) : C4	1	0
[96, 19]	(C3 : C16) : C2	1	0
[96, 21]	(C3 : C4) : C8	1	0
[96, 22]	C24 : C4	1	0
[96, 23]	(C3 : Q8) : C4	1	0
[96, 24]	C24 : C4	1	0
[96, 25]	C24 : C4	1	0
[96, 26]	C3 : (C4 . D8 = C4 . (C4 x C2))	1	0
[96, 27]	(C24 x C2) : C2	1	0
[96, 28]	(C24 x C2) : C2	1	0
[96, 29]	C3 : (C4 . D8 = C4 . (C4 x C2))	1	0

ID	Group structure	BDA	ci
[96, 30]	(C3 x (C8 : C2)) : C2	1	0
[96, 31]	C3 : (C2 . ((C4 x C2) : C2) = (C2 x C2) . (C4 x C2))	1	0
[96, 32]	(C3 x (C8 : C2)) : C2	1	0
[96, 33]	(C3 x D16) : C2	1	0
[96, 34]	(C3 : C16) : C2	1	0
[96, 35]	(C3 x Q16) : C2	1	0
[96, 36]	C3 : Q32	1	0
[96, 37]	(C2 x (C3 : C8)) : C2	1	0
[96, 38]	(C12 x C2) : C4	1	0
[96, 39]	(C2 x (C3 : C8)) : C2	1	0
[96, 40]	((C3 : C8) : C2) : C2	0	0
[96, 41]	((C2 x (C3 : C4)) : C2) : C2	0	0
[96, 42]	(C3 x Q8) : C4	1	0
[96, 43]	C3 : (C2 . ((C4 x C2) : C2) = (C2 x C2) . (C4 x C2))	0	0
[96, 44]	(C4 x (C3 : C4)) : C2	1	0
[96, 64]	((C4 x C4) : C3) : C2	1	0
[96, 65]	A4 : C8	1	0
[96, 66]	SL(2,3) : C4	1	0
[96, 67]	SL(2,3) : C4	1	0
[96, 70]	((C2 x C2 x C2 x C2) : C3) : C2	1	0
[96, 71]	((C4 x C4) : C3) : C2	0	0
[96, 72]	((C4 x C4) : C3) : C2	1	0
[96, 74]	((C8 x C2) : C2) : C3	1	0
[96, 76]	C12 : Q8	1*	0
[96, 77]	C3 : ((C2 x C2) . (C2 x C2 x C2))	1	0
[96, 79]	(C12 x C4) : C2	1	0
[96, 81]	(C12 x C4) : C2	1*	0
[96, 82]	(C12 x C4) : C2	1	0
[96, 83]	(C12 x C4) : C2	1	0
[96, 84]	(C4 x (C3 : C4)) : C2	1	0
[96, 85]	(C2 x (C3 : Q8)) : C2	1	0
[96, 86]	(C4 x (C3 : C4)) : C2	1	0
[96, 88]	(C2 x C4 x S3) : C2	1	0
[96, 89]	(C2 x C2 x C2 x S3) : C2	1*	0
[96, 90]	(C2 x C4 x S3) : C2	1	0
[96, 91]	(C2 x C4 x S3) : C2	1	0
[96, 92]	(C2 x (C3 : Q8)) : C2	1	0
[96, 93]	(C2 x C2 x (C3 : C4)) : C2	1	0
[96, 94]	(C3 : Q8) : C4	1	0
[96, 95]	C12 : Q8	1*	0
[96, 96]	C3 : ((C2 x C2) . (C2 x C2 x C2))	1	0
[96, 97]	C3 : ((C2 x C2) . (C2 x C2 x C2))	1	0
[96, 99]	(C4 x (C3 : C4)) : C2	1	0
[96, 100]	(C2 x C4 x S3) : C2	1	0
[96, 101]	(C2 x C4 x S3) : C2	1	0
[96, 102]	(C2 x C4 x S3) : C2	1	0
[96, 103]	(C2 x (C3 : Q8)) : C2	1	0
[96, 104]	(C3 x (C4 : C4)) : C2	1	0
[96, 105]	(C3 x (C4 : C4)) : C2	1	0
[96, 108]	(C24 x C2) : C2	1	0
[96, 111]	(C24 x C2) : C2	1	0
[96, 114]	(C8 x S3) : C2	1	0
[96, 115]	(C2 x D24) : C2	2*	0
[96, 116]	(C3 x (C8 : C2)) : C2	2*	0
[96, 118]	(D8 x S3) : C2	2	0
[96, 119]	(C8 x S3) : C2	1	0
[96, 121]	(D8 x S3) : C2	2*	0
[96, 122]	(Q8 x S3) : C2	2*	0
[96, 123]	(C8 x S3) : C2	1	0
[96, 125]	(C3 x Q16) : C2	2	0
[96, 126]	(C8 x S3) : C2	1	0
[96, 131]	(C2 x (C3 : Q8)) : C2	1	0
[96, 133]	(C4 x (C3 : C4)) : C2	1	0
[96, 136]	(C12 x C2 x C2) : C2	1	0
[96, 137]	(C12 x C2 x C2) : C2	1	0
[96, 139]	(C6 x D8) : C2	1	0

ID	Group structure	BDA	ci
[96, 142]	(C2 x C2 x (C3 : C4)) : C2	1	0
[96, 143]	(C2 x (C3 : Q8)) : C2	1	0
[96, 144]	(C2 x C2 x C2 x S3) : C2	1	0
[96, 145]	(C6 x D8) : C2	1	0
[96, 146]	(C2 x C2 x (C3 : C4)) : C2	1	0
[96, 147]	(C6 x D8) : C2	1	0
[96, 149]	(C6 x Q8) : C2	1	0
[96, 151]	(C3 : C4) : Q8	1	0
[96, 153]	(C6 x Q8) : C2	1	0
[96, 154]	(C6 x Q8) : C2	1	0
[96, 155]	(C2 x (C3 : C8)) : C2	1	0
[96, 156]	(C2 x D24) : C2	1	0
[96, 157]	(C2 x (C3 : C8)) : C2	1	0
[96, 158]	(C2 x (C3 : Q8)) : C2	1	0
[96, 160]	(C6 x C2 x C2 x C2) : C2	1	0
[96, 185]	A4 : Q8	1*	0
[96, 187]	(C2 x S4) : C2	1*	0
[96, 190]	(C2 x SL(2,3)) : C2	1	0
[96, 191]	(C2 . S4 = SL(2,3) . C2) : C2	1*	0
[96, 192]	(C2 . S4 = SL(2,3) . C2) : C2	1	0
[96, 193]	(SL(2,3) : C2) : C2	1*	0
[96, 195]	(C2 x C2 x A4) : C2	1	0
[96, 201]	(SL(2,3) : C2) : C2	1	0
[96, 202]	(C2 x SL(2,3)) : C2	1	0
[96, 203]	(C2 x C2 x Q8) : C3	0	0
[96, 204]	((C2 x D8) : C2) : C3	0	0
[96, 211]	(C6 x D8) : C2	1	0
[96, 214]	(C6 x Q8) : C2	1	0
[96, 216]	(D8 x S3) : C2	1*	0
[96, 217]	(Q8 x S3) : C2	1*	0
[96, 227]	((C2 x C2 x C2 x C2) : C3) : C2	1*	0
[98, 1]	D98	1*	0
[98, 4]	(C7 x C7) : C2	1*	0
[100, 1]	C25 : C4	1	0
[100, 3]	C25 : C4	0	0
[100, 7]	(C5 x C5) : C4	1	0
[100, 10]	(C5 x C5) : C4	0	0
[100, 11]	(C5 x C5) : C4	0	0
[100, 12]	(C5 x C5) : C4	0	0

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