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École doctorale de sciences mathématiques de Paris centre

Thèse de doctorat

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présentée par

Perla Azzi

Geometry of isotropy classes for representation of groups with applications in Mechanics of Materials

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co-dirigée par Julien Grivaux et Rodrigue Desmorat

Soutenue le 21 Avril 2023 devant le jury composé de :

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Abstract

This study revolves around linear representations of compact Lie groups and the study of the isotropy classes of such representations. The initial motivation of this work lays down in solving some problems in mechanics of materials where representations of compact groups, such as subgroups of O(3), are involved.

Isotropy classes of group representations are known to be semialgebraic sets characterized by polynomial invariants inequalities. In this thesis, we prove that, in fact, for any representation of compact Lie group, closed isotropy classes are algebraic sets. This result is motivated by several examples in mechanics. For instance, isotropy classes of SO(3)-representation on the space of second and fourth order harmonic tensors in mechanics are given by polynomial equations, which make them algebraic sets. Furthermore, we prove a theorem in invariant theory, about the rationality of invariants for compact Lie group representations. More specifically, for any representation of a compact Lie group G on a real vector space V and for any isotropy group H, any polynomial invariant of the representation of the normalizer $N(H)$ on the fixed point set V^H is indeed the restriction on V^H of a rational invariant of the initial representation of G on V. The latter assertion was already known under some restrictive conditions, such as in the case of algebraically closed fields and generic isotropies. In this work, the results are proven over $\mathbb{R}$ and with no further conditions.

In a second time, an effective method for determining the isotropy classes for reducible representations is proposed. This method is based on a binary operation between conjugacy classes of closed subgroups of a compact group, which has been introduced to obtain the isotropy classes of a direct sum of representations, if the isotropy classes are known for the irreducible factors. In the specific case of the three dimensional orthogonal group O(3), clips between some types of subgroups of O(3) have already been calculated. However, until now, clips between type II and type III subgroups were missing. Those are encountered in 3D coupled constitutive laws. In this thesis, we complete the clips tables by computing the missing clips. As an application, we obtain 25 isotropy classes for the standard O(3)-representation on the full 3D Piezoelectric law, which involves the three elasticity, piezoelectricity and permittivity constitutive tensors.

Another problem that has been encountered many times in mechanics is solved in this work using algebraic methods: given an experimental material with no specific isotropy, it is interesting to determine the closest isotropy of a contitutive tensor for this material. To solve such a problem, we used methods of polynomial optimization taking advantage of the characterization of the isotropy classes by polynomial covariants. Two polynomial optimization methods are presented to solve this question and applied to some constitutive laws in mechanics such as elasticity and piezoelectricity laws: one makes use of some effective algorithm based on real algebraic geometry

and theory of moments and the other one is an explicit calculation of critical points by an algebraic method called Euler-Lagrange method.

Keywords

Compact group representation, isotropy classes, constitutive law, polynomial optimization, continuum mechanics.

Résumé

Cette étude tourne autour des représentations linéaires des groupes de Lie compacts et de l'étude des classes d'isotropie de ces représentations. La motivation initiale de ce travail réside dans la résolution de certains problèmes en mécanique des matériaux où des représentations de groupes compacts, tels que les sous-groupes de O(3), sont impliqués.

Les classes d'isotropie des représentations de groupes sont connues pour être des ensembles semialgébriques caractérisés par des inégalités d'invariants polynomiaux. Dans cette thèse, nous prouvons que pour toute représentation d'un groupe de Lie compact, les classes d'isotropie fermées sont des ensembles algébriques. Ceci est motivé par de nombreux exemples en mécanique. Par exemple, les classes d'isotropie de la représentation de SO(3) sur l'espace des tenseurs harmoniques d'ordre 2 et 4 en mécanique sont données par des équations polynomiales, ce qui en fait des ensembles algébriques. De plus, nous prouvons un résultat en théorie des invariants, concernant la rationalité des invariants pour les représentations des groupes de Lie compacts. Plus précisément, pour toute représentation d'un groupe de Lie compact G sur un espace vectoriel réel V et pour tout groupe d'isotropie H, tout invariant polynomial de la représentation du normalisateur $N(H)$ sur l'ensemble des points fixes V^H est bien la restriction sur V^H d'un invariant rationnel de la représentation initiale de G sur V. Cette dernière affirmation était déjà connue sous certaines conditions restrictives, comme dans le cas de corps algébriquement clos et d'isotropies génériques. Dans ce travail, les résultats sont prouvés sur $\mathbb{R}$ et sans autres conditions.

Dans un deuxième temps, une méthode pour déterminer les classes d'isotropie pour les représentations réductibles est proposée. Cette méthode est basée sur une opération binaire entre les classes de conjugaison des sous-groupes fermés d'un groupe compact, qui a été introduite pour obtenir les classes d'isotropie d'une somme directe de représentations, si les classes d'isotropie sont connues pour les facteurs irréductibles. Dans le cas spécifique du groupe orthogonal tridimensionnel O(3), les clips entre certains types de sous-groupes de O(3) ont déjà été calculés. Cependant, jusqu'à présent, il manquait les clips entre les sous-groupes de type II et de type III. Ceux-ci apparaissent dans les lois constitutives couplées en 3D. Dans cette thèse, nous complétons les tables de clips en calculant les clips manquants. Comme application, nous obtenons 25 classes d'isotropie pour la représentation standard O(3) sur la loi piézoélectrique 3D complète, qui implique les trois tenseurs constitutifs d'élasticité, de piézoélectricité et de permittivité.

Un autre problème rencontré à de nombreuses reprises en mécanique est résolu dans ce travail en utilisant des méthodes algébriques : étant donné un matériau expérimental sans isotropie spécifique, il est intéressant de déterminer l'isotropie la plus proche d'un tenseur constitutif pour ce matériau. Pour résoudre un tel problème, nous avons utilisé des méthodes d'optimisation

polynomiale en tirant profit de la caractérisation des classes d'isotropie par des covariants polynomiaux. Deux méthodes d'optimisation polynomiale sont présentées pour résoudre cette question et appliquées à certaines lois constitutives en mécanique telles que les lois d'élasticité et de piézoélectricité : l'une utilise un algorithme effectif basé sur la géométrie algébrique réelle et la théorie des moments et l'autre est un calcul explicite des points critiques par une méthode algébrique appelée méthode d'Euler-Lagrange.

Mots-clés

Représentation de groupe compact, classes d'isotropie, loi de comportement, optimisation polynomiale, mécanique des milieux continus.

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Introduction

This PhD thesis is part of the project 80PRIME GAMM (Géométrie algébrique complexe/réelle et mécanique des matériaux) co-funded by two institutes of French CNRS,

(*i*) the mathematics institute INSMI (*Institut National des Sciences Mathématiques et de leurs Interactions*) and

(*ii*) the engineering institute INSIS (*Institut des Sciences de l'Ingénierie et des Systèmes*).

It straddles two research laboratories: IMJ-PRG (*Institut de Mathématiques de Jussieu - Paris Rive Gauche*) and LMPS (*Laboratoire de Mécanique Paris Saclay*). The main purpose of this thesis is to solve mathematical conjectures and mechanical problems arising from Continuum Mechanics using, in particular, real and complex algebraic geometry.

Mechanical motivation

In physics, the behavior of a material is described using constitutive laws and such laws are modeled using tensors. The tensor formulation of linear constitutive laws plays an important role in various physical theories, ranging from electromagnetism to continuum mechanics (see for instance [10]):

- In the framework of linear elasticity, the stress tensor $\boldsymbol{\sigma}$ (of order 2) and the strain tensor $\boldsymbol{\varepsilon}$ (of order 2) of a material are related by the generalized Hooke's law $\boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\varepsilon}$. The fourth-order tensor $\mathbf{E}$ is called the elasticity tensor.

- In the framework of piezoelectricity, the electric displacement tensor $\boldsymbol{d}$ (of order 1) and the stress tensor $\boldsymbol{\sigma}$ (of order 2) are related by the tensorial constitutive equation $\boldsymbol{d} = \mathbf{P} : \boldsymbol{\sigma}$, where the piezoelectric tensor $\mathbf{P}$ is a third-order tensor.

In these tensorial formulations, the material behavior is described by $\mathbb{R}$-valued tensors ($\mathbf{E}$ and $\mathbf{P}$). However, such a correspondence is not univocal: it depends on the orientation of the material in space. From a mathematical point of view, this corresponds to the action of the orthogonal group O(3) on the tensor space under study. Thus, in order to recognize a material, it is necessary to identify the orbit of the associated set of constitutive tensors. Besides, it is also important to take into account the symmetries of the material [25]. Appealing to Curie principle: –*"the*

symmetries of the causes are to be found in the effects"–, a symmetry of a constitutive tensor is often expected in mechanical applications, by observing the micro-structure of a material. For instance, the elasticity tensor of a single crystal alloy with cubic crystal network is expected to be cubic (conjugacy class $[\mathbb{O}]$), the piezoelectric tensor of an aluminum nitrite (AlN) alloyed with rocksalt transition metal nitrites is expected to become cubic (conjugacy class $[\mathbb{O}^-]$) for a high chromium concentration [74].

The questions related to material symmetries can be formulated in the language of the representation theory of groups ([13, 105, 44, 14]). We can classify the constitutive tensors according to their invariance under some O(3)-subgroup, and gather them in sets called *isotropy strata*. In mechanics, since the considered groups are compact Lie groups, the space of the considered tensors decomposes into a finite disjoint union of *isotropy strata*. Each of these strata thus corresponds to a given symmetry, indexed by a conjugacy class $[H]$ of a closed subgroup H of G.

This thesis is devoted to problems posed by solid mechanics and formulated in the geometrical framework of isotropy strata of a compact Lie group representation.

Problematics

Geometry of isotropy strata for compact Lie group representations

The geometrical structure of isotropy strata for a group representation G on a real vector space V can be deduced from the geometry of the orbit space V/G. The initial observation is that the space of orbits V/G can be described directly using the invariant algebra $\mathbb{R}[V]^G$. In fact, if G is a compact Lie group, the algebra of G-invariant polynomials is known to separate the orbits [1, Appendix C]. Consequently, if $\{J_1, J_2, \ldots, J_N\}$ is a set of polynomial invariants which separate the G-orbits, then the map

$$J : v \mapsto \big(J_1(v), J_2(v), \ldots, J_N(v)\big)$$

induces an algebraic homeomorphism $\tilde{J}$ between the *orbit space* V/G and $J(V) \subset \mathbb{R}^N$, which is a semialgebraic subset of $\mathbb{R}^N$. This link between the invariant algebra and the orbit space is initially described by Abud–Sartori [1] and then clearly established by Procesi–Schwarz [95]. More precisely, the semialgebraic description of V/G is expressed using the positivity of a matrix with entries the differentials of the G-invariant functions. This matrix is called the Bézout matrix (see [95]) or the Hermite matrix (see [23, section 1.4.1]). A rational parametrization for the orbit space using invariant functions has been studied by Sartori-Valente in [101]. A recent study on this link was then initiated by Auffray-Kolev-Petitot [2], restricting to the case of an irreducible representation of $\mathrm{SO}(3, \mathbb{R})$. In [2], Auffray-Kolev-Petitot reduced the study of orbit space, in a non trivial particular case, by considering the representation of the normalizer $N(H)$, for H an isotropy subgroup of G, on the subspace of fixed points V^H of V.

Beyond the semialgebraic structure of the isotropy strata, it was observed, in some cases in mechanics of materials, that isotropy strata can be characterized explicitly by polynomial equations. For instance, in [38], most of the isotropy strata of the SO(2)-representation on the space of elasticity tensors are given by polynomial equations. Moreover, recently, the exploitation

of covariants, geometrically richer than the invariants, allowed to obtain explicit polynomial equations of the eight strata of the SO(3)-representation on the space of harmonic tensors of order 4 (see [91]). This characterization of the isotropy strata by polynomial equations in some specific cases, brings up questions about the algebraic structure of strata in more general contexts. An important result of this thesis is that, for any representation of compact Lie group on a real vector space V, *closed isotropy strata are real algebraic subsets of* V, being an irreducible component of the real locus of an algebraic complex variety (Theorem 1.1 of chapter 2).

Rationality of polynomial invariants for compact Lie group representations

It was observed in [2], on an example issued from mechanics, that polynomial invariants for the restricted representation of the normalizer of an isotropy subgroup H of the group G on the fixed point set V^H could be expressed rationally using polynomial invariants of the original representation of the group G on V. In other words, when H is an isotropy subgroup of G, the field of G-invariants on V is isomorphic to the field of $N(H)$-invariants on V^H. To illustrate this assertion, consider the example of the natural representation of the rotation group $\mathrm{SO}(3,\mathbb{R})$ on the vector space of traceless symmetric matrices with real coefficients

$$\rho(g)(A) = gAg^{-1}, \qquad A \in \mathbb{H}^2(\mathbb{R}^3), \quad g \in \mathrm{SO}(3,\mathbb{R}).$$

For this representation, there are exactly three isotropy strata of representative groups $\mathbb{D}_2$ (three distinct eigenvalues), O(2) (two distinct eigenvalues) and SO(3) (only one eigenvalue). The fixed point set for the second isotropy subgroup O(2) is provided by the linear subspace

$$V^{\mathrm{O}(2)} = \left\{A \in V;\ gAg^{-1} = A, \quad \forall g \in \mathrm{O}(2)\right\} = \left\{\mathrm{diag}(-\lambda, -\lambda, 2\lambda);\ \lambda \in \mathbb{R}\right\}.$$

Then, one can check that $\lambda = \frac{I_3}{I_2}$, where $I_2 = \mathrm{tr}\, A^2$ and $I_3 = \mathrm{tr}\, A^3$ are a generating set of the invariant algebra

$$\mathbb{R}[\mathbb{H}^2(\mathbb{R}^3)]^{\mathrm{SO}(3,\mathbb{R})}.$$

Similar results can be found in the literature but under different hypotheses. In fact, the isomorphism between the invariant field for the representation (V, G) and the invariant field for the restricted representation $(V^H, N(H))$ is a consequence of the slice method used for solving the rationality problem of the invariant field (see [29, 22]). The rationality problem consists in studying the conditions on the representation (V, G), under which the field of invariants $K(V)^G$ is purely transcendental over K. This is a very old problem: it was mentioned in 1911 in [16] (p.360), then, in 1913, Noether [83] posed the problem in the form of a conjecture. In 1915, Fisher [35] proved that the field of invariants $K(V)^G$ is purely transcendental over K when G is an abelian group. Also, Maeda proved the result for the alternating group A_5 [71]. However, it is not always true. For instance, $K(V)^G$ is not purely transcendental if G is a finite group [100]. Moreover, counter-examples to Noether's conjecture were given in the case of non-algebraically closed fields [76] (see also [106, 21, 99]). The question is still open in many cases, for instance in the case where the group G is connected.

The isomorphism between the two invariant fields $K(V)^G$ and $K(V^H)^{N(H)}$ was proved for

several cases with the purpose of solving the rationality problem by the slice method. For instance, in order to prove the rationality of the invariant field for the group $SL_2(\mathbb{C})$ acting on the binary forms of degree $2n$, Bogomolov-Katsylo in [56, 57, 11] and later Maeda in [72], proved that $\mathbb{C}(V)^G$ is isomorphic to $\mathbb{C}(V^H)^{N(H)}$ (for H generic). Miyata [79] and later Vinberg [109] proved the rationality of the orbit space V/G for solvable connected algebraic groups by applying the slice method looking for the slice W such that $N(W)$ is a solvable connected subgroup (see also [94, section 2.9]). The result was also proven in [41] for the spinor group and in [46, 47] for finite groups of monomial automorphisms. The rationality problem has a positive answer in many cases where the isomorphism $K(V)^G \simeq K(V^H)^{N(H)}$ is used to prove it (for more details see [22]).

In addition, Luna in [69] and then Luna and Richardson in [70, theorem 4.2] proved that, for a linear action of a reductive group G on an affine variety V (so in particular for a linear representation of G), the restriction map $K[V^H] \to K[V]$ maps $K[V]^G$ isomorphically onto $K[V^H]^{N(H)/H}$ when K is an algebraically closed field and H is a generic isotropy (see also [104]).

In this thesis, we prove that there is surjective morphism between the two invariant fields over $\mathbb{R}$ and for any isotropy subgroup H, not only the generic one, that is: *for any representation of a compact Lie group G on a real vector space V and for any isotropy subgroup H, the restriction map $\mathbb{R}[V] \to \mathbb{R}[V^H]$ induces a surjective morphism*

$$S : \mathbb{R}(V)^G \dashrightarrow \mathbb{R}(V^H)^{N(H)},$$

between the invariant fields of (V, G) that are rationally defined on V^H, and of those of $(V^H, N(H))$.

The proof appeals to Popov and Vinberg orbits separating theorem ([94, lemma 2.1]) and to results on the geometry of orbits by Luna [69] and Richardson [70]. Popov and Vinberg's theorem states that a separating set is a generating set of $\mathbb{C}(V^H)^{N(H)}$. Note that the latter theorem is wrong in the real setting. For instance, in the case of the real representation of the trivial group $G = \{e\}$ on the real space $V = \mathbb{R}$, the invariant field is given by $\mathbb{R}(V)^G = \mathbb{R}(x)$. The polynomial $p(x) = x^3$ separates all the orbits but is not a generator of $\mathbb{R}(V)^G$. For this reason, a detailed theory on the complexification of a real linear representation of a compact Lie group is fully provided in chapter 2.

Calculating isotropy strata for a compact Lie group representation

Finding the isotropy strata has always been a difficult problem. Classifying materials according to their symmetries goes back at least to the work of Lord Kelvin ([107], [58]). From then, many researchers devoted a great effort to the problem, especially for SO(3) and O(3) tensorial representations (used to model constitutive laws in mechanics). For instance, concerning the fourth-order elasticity tensor [45, 24, 103, 112, 17], it was only in 1996 that Forte and Vianello [37] proved that there exists exactly eight symmetry classes. Inspired by the observation of Khatkevich ([59]), Forte-Vianello clarified the mathematical problem about the symmetry classes of an elasticity tensor. They removed the link with crystallographic point groups, which was extremely confusing and lead to the false conjecture that there were ten symmetry classes.

Following Forte and Vianello, similar results were obtained for other constitutive tensor spaces ([38, 66]). For instance, sixteen isotropy classes were obtained for the piezoelectricity tensor (a third-order tensor) [84, 113, 111, 82, 114].

Besides these results on symmetry classes in continuum mechanics, the subject has also been active in the mathematical community. First, it was interesting to see whether there is a finite number of isotropy strata or not. When the group is not finite, the existence of a finite number of isotropy classes was first conjectured by Montgomery ([32]). Later, Mostow extended the result for a compact Lie group acting (not necessarily in a differentiable way) on a compact manifold [81], using results of Floyd [36] (see also [73, 13]). After that, isotropy classes of *irreducible representations* for SO(3)-linear representations were obtained by Michel [78]. Then, Ihrig and Golubitsky [53] extended the result of Michel to the case of O(3)-irreducible representations. However, Forte-Vianello approach requires rather refined calculations and reasoning to establish the classification. This complexity makes it difficult to apply to more involved situations, such as constitutive tensors of order greater than 4, or coupled constitutive laws involving a family of tensors [54, 33]. A systematic way to calculate such isotropy classes was proposed by Chossat and Guyard in [18] for a direct sum of two irreducible SO(3)-representations. To do so, they introduced a binary operation on conjugate SO(3)-subgroups that allows one to compute the set of isotropy classes of a direct sum $V = V_1 \oplus V_2$ of linear representations of a group G (if the isotropy classes for each individual irreducible representation are known). Inspired by Chossat and Guyard, Olive and coauthors used this operation, called *clips operation*, to complete and systemize the initial work of Chossat et al ([87], [88], [86] and [89]). Clips form a binary operation on the set of conjugacy classes of subgroups of a compact group G. It comes down to calculate the intersections between two subgroups H_1 and gH_2g^{-1} for $g \in G$. In the case of the group O(3), clips operation between most of O(3)-subgroups are computed in [18] and [86], except for the clips between type II and type III O(3)-subgroups. Those are nevertheless encountered in practice, such as in the coupled Piezoelectricity law, where the representations of O(3) on three different constitutive tensor spaces are involved, namely the fourth-order elasticity tensor, the third-order piezoelectricity tensor and the second-order permittivity tensor.

We complete in the present work the clips tables of O(3) *by computing the missing type II/type III clips*. As an application of this result, we obtain *25 isotropy strata for the coupled Piezoelectricity law*. We also address the coordinate-free characterization of isotropy strata by polynomial covariants [38, 7, 98, 12, 2, 91]

Distance of a constitutive tensor to an isotropy stratum

An important problem in mechanics is the problem of determining the distance of a constitutive tensor to an isotropy stratum [42, 39]. A measured constitutive tensor exhibits, in general, no material symmetry. However, in engineering applications, a measured tensor may have an expected symmetry due to the microstructure of the corresponding material (appealing to Curie principle). Finding the closest symmetry stratum to an experimental tensor is important in practice, since it allows to reduce the number of material constants. A natural question can then be asked: "What is the closest tensor having a given symmetry class, to an experimental

measured tensor?" In order to answer this question, one needs to calculate the distance

$$d(\mathbf{T}_0, \overline{\Sigma}) = \min_{\mathbf{T} \in \overline{\Sigma}} \|\mathbf{T}_0 - \mathbf{T}\|^2$$

between the measured tensor $\mathbf{T}_0$ and the closed isotropy stratum $\overline{\Sigma}$ representing the expected symmetry of $\mathbf{T}_0$ and, then, deduce the corresponding minimizer.

This notion of distance to symmetry classes was first introduced in mechanics by Gazis and coauthors, in 1963, using orthogonal projections of elasticity tensors on the isotropy stratum. Following Gazis, many authors considered the calculation of the distance to find the closest tensor having a specific symmetry to an experimental one [40, 80, 15, 61, 28, 27, 26, 60, 93]). In [40], François used the pole figures to deduce the symmetry class of an elasticity tensor. He considered an iterative numerical method based on the simplex method for minimization problems, parameterized by Euler angles, which turns the problem into a non-polynomial one. Other authors followed François, however they did not formulate the distance to a symmetry stratum as a polynomial optimization problem, so that the problems they had to solve (numerically) had many local minima and several global minima, making the computations of the solutions difficult.

In order to solve the distance problem, we take advantage of the fact that the isotropy strata can be described by polynomial equations, and *formulate the distance of a constitutive tensor to an isotropy stratum as a polynomial optimization problem*, which consists in minimizing or maximizing a polynomial function under some polynomial constraints.

In chapter 5 of this manuscript, we investigate a polynomial optimization method designed by Lasserre and coworkers [65] to solve our problem, thanks to our formulation of the distance problem as a polynomial optimization problem. This method consists in building a hierarchy of relaxed semidefinite problems converging to the optimal solution under some hypothesis on the constraints set. This method is implemented in a software called GloptiPoly [48, 49, 65]. However, Lasserre's method deals with problems in terms of number of variables and degree of constraints which restricts its application to some specific constitutive laws. Using this method, we were able to find the closest cubic tensor to some experimental tensors for elasticity and piezoelectricity laws.

On the other hand, in order to minimize a polynomial function under polynomial constraints, one can also use analytical methods such as Euler-Lagrange method. It consists in formulating the constrained problem into an unconstrained one using Lagrange multipliers and then finding the critical points of the considered function by solving a system of polynomial equations [9, 55, 63]. However, this method requires that the set of constraints to be a submersion, which is far from being satisfied by all the situations with mechanical interest. In chapter 6, this method, combined with the computation of a Gröbner basis, allows to solve the distance to cubic elasticity. In addition, we determine the closest pair of cubic elasticity and plasticity tensor to an experimental one (*i.e.* in the case of the coupled elasto-plasticity law), a problem that could not be solved using Lasserre's algorithm since it involves more variables.

To conclude, this thesis emphasizes the fruitful links between Mechanics of Materials and

Algebraic Geometry. While mechanics keeps inspiring conjectures in algebraic geometry, tools from algebraic geometry keep being applied to solve mechanics problems.

Outline

This manuscript is organized as follows. In chapter 1, we provide basic materials about group actions on a set focusing on compact Lie group representations. We recall some key properties of linear representations of compact Lie groups and we introduce some definitions and questions related to isotropy classes, stratification and geometry of orbit spaces. We provide proofs to some known theorems, such as the principal orbit theorem. In the end of this chapter, we present the theory of invariants and covariants, examples and counter-examples are exposed in order to illustrate some mechanical and mathematical notions all along the chapter.

In chapter 2, we study *the geometry of isotropy strata for compact Lie group representations*. We answer a ten-year-old conjecture on the rationality of the invariants of compact Lie group representations, deduced from observations made in the case of SO(3)-representations on tensor spaces in continuum mechanics. Moreover, we prove a result about the algebraicity of the isotropy strata:

- For any representation of a compact Lie group G on a real vector space V and for any isotropy group H, the polynomial invariants of the representation of the normalizer $N(H)$ on the fixed point set V^H can be written rationally in terms of the polynomial invariants of the initial representation of G on V.
- Under the same assumptions, closed isotropy strata are proved to be algebraic sets.

Complexification of compact Lie groups and real representations is needed. For this purpose, a detailed theory on complexification is provided in this chapter.

In chapter 3, we specify a number of general results from chapter 1 to the case of linear representations of the groups O(3) and SO(3). First, we calculate a detailed list of O(3)-subgroups with their corresponding generators (in Table 3.1). Second, we discuss the harmonic decomposition of tensor spaces, which consists in decomposing tensor representations into irreducible spaces (a model of which is given by so-called harmonic tensor spaces). On one hand, we give isotropy classes for some O(3)-irreducible representations and we give a polynomial characterization of isotropy classes in the case of SO(3)-representation on harmonic spaces of order 4 (theorem 3.2.7). On the other hand, we introduce an effective method to *find the isotropy classes for reducible representations*. For this purpose, we use the clips operation on the isotropy classes and give the result of these clips operations on the closed subgroups of SO(3) as well as on the closed subgroups of O(3) which were not all calculated before. As a consequence, in this chapter, we provide a complete table of the clips operations between all types of O(3)-subgroups (Table 3.2 and Table 3.3) using a theorem (3.5.2) that helped us reduce the complexity of the calculations. Using these results, we deduce the isotropy classes of any reducible O(3)-tensor representation and we illustrate this in the case of Piezoelectricity coupled law in chapter 4.

In chapter 4, we use the clips calculations of chapter 3 to deduce the isotropy classes in the case of the coupled Piezoelectricity law which involves O(3)-representations on three tensor

spaces: elasticity, piezoelectricity and permittivity. We start by introducing the Piezoelectricity coupled law and then we give a detailed description of the O(3)-representation on elasticity and piezoelectricity tensor spaces. Using the isotropy classes of each of the three representations involved and the clips operation calculated in chapter 3, we find 25 isotropy classes (theorem 4.4.1) for the Piezoelectricity coupled law.

In the last two chapters, we solve the problem of *finding the closest constitutive tensor having a specific symmetry to an experimental one by calculating the distance of the tensor to the chosen symmetry class. For that, we use polynomial optimization methods.* In chapter 5, we apply Lasserre's algorithm for solving polynomial optimization problems to some numerical example in the case of elasticity and piezoelectricity laws. In chapter 6, we use Euler-Lagrange method to minimize our constrained problem by calculating the Euler-Lagrange equations. As an application, we apply this method in the case of elasticity and coupled elasto-plasticity laws.

Chapter 1

Geometry representation of compact Lie groups

In this chapter, fundamental concepts in representation theory will be introduced to describe the orbit space of the action of a compact Lie group on a vector space.

1.1 Action of a group on a set

1.1.1 Definition and properties

Let G be a group and V a set. An *action* of G on V is a map

$$\begin{aligned} G \times V &\to V \\ (g, \boldsymbol{v}) &\mapsto g \cdot \boldsymbol{v} \end{aligned}$$

satisfying the following properties

1. For all $g, h \in G$ and $\boldsymbol{v} \in V$, $g \cdot (h \cdot \boldsymbol{v}) = gh \cdot \boldsymbol{v}$;
2. For all $\boldsymbol{v} \in V$, $e \cdot \boldsymbol{v} = \boldsymbol{v}$ where e is the identity of G.

Remark 1.1.1. *This definition corresponds to a left action but a group can also acts on the right. In this manuscript, we only consider left actions.*

Example 1.1.2. *Any group acts on itself by left multiplication. In other words, G acts on $V = G$ by $g \cdot h = gh$ where $g, h \in G$. A closely related action is given by right multiplication $g \cdot h = hg^{-1}$ if $g, h \in G$. The use of the inverse is required so the first property of being an action is satisfied.*

Suppose that we have an action of G on V, we say that a subset W of V is *G-stable* if

$$\forall g \in G,\ \forall \boldsymbol{v} \in W,\ g \cdot \boldsymbol{v} \in W, \tag{1.1}$$

and we say that W is *G-invariant* if

$$\forall g \in G,\ \forall \boldsymbol{v} \in W,\ g \cdot \boldsymbol{v} = \boldsymbol{v}. \tag{1.2}$$

Example 1.1.3. *Consider the action of the rotation group $SO(2)$ on $\mathbb{R}^2$ defined by*

$$g \cdot (x, y) := (x\cos(\theta) - y\sin(\theta), x\sin(\theta) + y\cos(\theta))$$

for $g \in SO(2)$ and $(x, y) \in \mathbb{R}^2$. Any circle $\left\{x^2 + y^2 = r^2\right\}$ centered at the origin is a SO(2)*-stable set of $\mathbb{R}^2$.*

To an action of a group G on a set V is associated the group morphism

$$\varphi : G \to \mathrm{Bij}(V)$$

defined by, if $g \in G$, for all $\boldsymbol{v} \in V$, $\varphi(g)(\boldsymbol{v}) = g \cdot \boldsymbol{v}$ ($\mathrm{Bij}(V)$ denotes the group of bijections of V). The kernel of an action is the kernel of the associated morphism φ consisting of the elements $g \in G$ that fix all the elements of V. It is defined by

$$K = \{g \in G \mid \forall \boldsymbol{v} \in V,\ g \cdot \boldsymbol{v} = \boldsymbol{v}\}.$$

K is a closed normal subgroup of G.

Definition 1.1.4. *Let G be a group acting on a set V. We say that*

1. *G acts* faithfully *on V (or that the action of G is faithful) if its kernel K is trivial i.e. there is no element in G, except e, that fixes all the elements of V.*
2. *G acts* transitively *on V (or that the action of G is transitive) if $\forall \boldsymbol{v}, \boldsymbol{w} \in V$, $\exists g \in G$; $\boldsymbol{w} = g \cdot \boldsymbol{v}$ i.e. all the elements of V are related to each other by the action.*
3. *G acts* freely *on V (or that the action of G is free) if $\forall \boldsymbol{v} \in V$, $\forall g \in G$, $g \cdot \boldsymbol{v} = \boldsymbol{v} \implies g = e$ i.e. for any element of V, there is no element in G, except e, that fixes it.*

Remark 1.1.5. *A free action is faithful.*

Lemma 1.1.6. *Any (unfaithful) action of a group G on a set V defines a faithful action of the group G/K on V, where K is the kernel of the action.*

1.1.2 The orbit space

Given an action of a group G on a set V, an equivalence relation can be defined on V. For $\boldsymbol{v}_1, \boldsymbol{v}_2 \in V$, we define "$\sim$" as follows

$$\boldsymbol{v}_1 \sim \boldsymbol{v}_2 \iff \exists g \in G;\ \boldsymbol{v}_1 = g \cdot \boldsymbol{v}_2. \tag{1.3}$$

For $\boldsymbol{v} \in V$, the equivalence class of $\boldsymbol{v}$ is called the *G-orbit* of $\boldsymbol{v}$ and is denoted by $G \cdot \boldsymbol{v}$:

$$G \cdot \boldsymbol{v} := \{g \cdot \boldsymbol{v},\ g \in G\}. \tag{1.4}$$

The G-orbits form a partition of V and the space of all G-orbits of V is the *orbit space* denoted by V/G.

Remark 1.1.7. *We consider the projection map*

$$\pi : \ V \to V/G.$$

When V is a topological set, the orbit space V/G is equipped with the quotient topology induced from the topology on V:

$$U \subset V/G \text{ is open if and only if } \pi^{-1}(U) \text{ is open in } V.$$

The map π is open with respect to this topology.

1.1.3 Orbit types

If G acts on V and $\boldsymbol{v} \in V$, the set of elements of G fixing $\boldsymbol{v}$ is a subgroup of G, called the stabilizer of $\boldsymbol{v}$, and denoted by $G_{\boldsymbol{v}}$:

$$G_{\boldsymbol{v}} := \{g \in G;\ g \cdot \boldsymbol{v} = \boldsymbol{v}\}.$$

For the action of a topological group G on a topological set V, $G_{\boldsymbol{v}}$ is a closed subgroup of G ($G_{\boldsymbol{v}} = \pi_{\boldsymbol{v}}^{-1}(\{\boldsymbol{v}\})$ where $\pi_{\boldsymbol{v}} : G \to V$; $\pi_{\boldsymbol{v}}(g) = g \cdot \boldsymbol{v}$). $G_{\boldsymbol{v}}$ is called the *isotropy subgroup* (or *symmetry group*) of $\boldsymbol{v}$. We can remark that isotropy groups of elements of a same orbit are conjugate:

Lemma 1.1.8. *For any $\boldsymbol{v} \in V$ and any $g \in G$, we have*

$$G_{g \cdot \boldsymbol{v}} = g G_{\boldsymbol{v}} g^{-1}.$$

For $\boldsymbol{v} \in V$, we consider the orbit map $\rho_{\boldsymbol{v}}$ defined as follows:

$$\begin{aligned} \rho_{\boldsymbol{v}} : G &\to G \cdot \boldsymbol{v} \\ g &\mapsto g \cdot \boldsymbol{v}. \end{aligned}$$

The map $\rho_{\boldsymbol{v}}$ is surjective by definition of $G \cdot \boldsymbol{v}$ but not necessarily injective. Indeed, if $g, h \in G$, $g \cdot \boldsymbol{v} = h \cdot \boldsymbol{v} \iff g^{-1}h \in G_{\boldsymbol{v}}$, that is $h \in gG_{\boldsymbol{v}}$. This shows that $\rho_{\boldsymbol{v}}$ is injective if and only if $G_{\boldsymbol{v}} = \{e\}$ that is when the action is free on $\boldsymbol{v}$ (see definition 1.1.4). Consequently, there is a unique bijective mapping

$$G/G_{\boldsymbol{v}} \xrightarrow{\sim} G \cdot \boldsymbol{v}. \tag{1.5}$$

Next, we define another equivalence relation on V. For this we need the following definition.

Definition 1.1.9. *If ρ_1 and ρ_2 are two actions of G on two spaces V and W, then a mapping $\phi : V \to W$ is G-*equivariant *if*

$$\forall g \in G,\ \phi \circ \rho_1(g) = \rho_2(g) \circ \phi.$$

For $\boldsymbol{v}_1, \boldsymbol{v}_2 \in V$, we define "$\approx$" as follows:

$$\boldsymbol{v}_1 \approx \boldsymbol{v}_2 \iff \text{there exists a } G\text{-equivariant bijection } \phi : G \cdot \boldsymbol{v}_1 \to G \cdot \boldsymbol{v}_2. \tag{1.6}$$

$\approx$ is an equivalence relation and we denote the equivalence classes, called the *orbit types* of V, by:

$$V_{\boldsymbol{v}}^{\approx} = \{\boldsymbol{w} \in V \mid \boldsymbol{v} \approx \boldsymbol{w}\}. \tag{1.7}$$

In the same manner, a preorder can be defined on V,

$$\boldsymbol{v}_1 \precsim \boldsymbol{v}_2 \iff \text{there exists a } G\text{-equivariant map } \phi : G \cdot \boldsymbol{v}_1 \to G \cdot \boldsymbol{v}_2 \tag{1.8}$$

and we write

$$V_{\boldsymbol{v}}^{\precsim} = \{\boldsymbol{w} \in V \mid \boldsymbol{v} \precsim \boldsymbol{w}\}.$$

Lemma 1.1.10. *[30, lemma 2.6.2] For $\boldsymbol{v}_1, \boldsymbol{v}_2 \in V$, we have*

1. *$\boldsymbol{v}_1 \approx \boldsymbol{v}_2$ if and only if $G_{\boldsymbol{v}_1}$ is conjugate to $G_{\boldsymbol{v}_2}$ within G, that is, there exists $g \in G$ such that $G_{\boldsymbol{v}_1} = gG_{\boldsymbol{v}_2}g^{-1}$.*

2. *$\boldsymbol{v}_1 \precsim \boldsymbol{v}_2$ if and only if $G_{\boldsymbol{v}_1}$ is conjugate to a subgroup of $G_{\boldsymbol{v}_2}$ within G, that is, there exists $g \in G$ such that $G_{\boldsymbol{v}_1} \subset gG_{\boldsymbol{v}_2}g^{-1}$.*

Proof. 1. Suppose that $\boldsymbol{v}_1 \approx \boldsymbol{v}_2$ then there exists a G-equivariant bijection ϕ from $G \cdot \boldsymbol{v}_1$ to $G \cdot \boldsymbol{v}_2$. Then, there exists $g \in G$ such that $\phi(\boldsymbol{v}_1) = g \cdot \boldsymbol{v}_2$ and $G_{\phi(\boldsymbol{v}_1)} = G_{\boldsymbol{v}_1}$. We deduce that $G_{\boldsymbol{v}_1} = gG_{\boldsymbol{v}_2}g^{-1}$. The converse can be deduced from the bijection in (1.5).

2. Suppose that $\boldsymbol{v}_1 \precsim \boldsymbol{v}_2$ then there exists a G-equivariant map ϕ from $G \cdot \boldsymbol{v}_1$ to $G \cdot \boldsymbol{v}_2$. We have $\phi(\boldsymbol{v}_1) \in G \cdot \boldsymbol{v}_2$, so $\phi(\boldsymbol{v}_1) = g' \cdot \boldsymbol{v}_2$ for some $g' \in G$. Let $h \in G_{\boldsymbol{v}_1}$, then $h \cdot \boldsymbol{v}_1 = \boldsymbol{v}_1$. Applying ϕ, we get $\phi(h \cdot \boldsymbol{v}_1) = \phi(\boldsymbol{v}_1) = g' \cdot \boldsymbol{v}_2$ which implies $hg' \cdot \boldsymbol{v}_2 = g' \cdot \boldsymbol{v}_2$ ($\phi(h \cdot \boldsymbol{v}_1) = h \cdot \phi(\boldsymbol{v}_1)$). Hence $h \in g'G_{\boldsymbol{v}_2}g'^{-1}$. For the converse implication, assume that there exists $g \in G$ such that $G_{\boldsymbol{v}_1} \subset gG_{\boldsymbol{v}_2}g^{-1}$. We define $\phi : G \to G \cdot \boldsymbol{v}_2$ by $\phi(g') = g'g \cdot \boldsymbol{v}_2$ if $g' \in G$. The map ϕ is G-equivariant and factors through $G \cdot \boldsymbol{v}_1$ (which is bijective to $G/G_{\boldsymbol{v}_1}$ by (1.5)) via the orbit map. Indeed, if $g_1 \in G_{\boldsymbol{v}_1} \subset gG_{\boldsymbol{v}_2}g^{-1}$ then $g_1 = gg_2g^{-1}$ where $g_2 \in G_{\boldsymbol{v}_2}$ and $\phi(g'g_1) = \phi(g')$.

□

1.1.4 Fixed point set and isotropy classes

For a subgroup H of G, we gather all the elements $\boldsymbol{v} \in V$ fixed by the elements of H in a set called *H-fixed point set*, denoted by V^H:

$$V^H = \{\boldsymbol{v} \in V \mid \forall h \in H,\ h \cdot \boldsymbol{v} = \boldsymbol{v}\}.$$

Let H be a subgroup of G, the conjugacy class of H, denoted by $[H]$, is given by

$$[H] = \left\{gHg^{-1},\ g \in G\right\}.$$

The *isotropy class* of an element $\boldsymbol{v} \in V$ is the conjugacy class of its isotropy group. In other terms,

$$\boldsymbol{v}_1, \boldsymbol{v}_2 \in V \text{ have the same isotropy class iff } \exists g \in G \ / \ G_{\boldsymbol{v}_2} = g G_{\boldsymbol{v}_1} g^{-1}.$$

Given a closed subgroup H of G, we say that the conjugacy class $[H]$ of H in G is an *isotropy class* (or an *orbit type*) if there exists an element $\boldsymbol{v}$ such that $[H] = [G_{\boldsymbol{v}}]$.

"Having the same isotropy class" is an equivalence relation defined on V which is the same (by lemma 1.1.10) as the equivalence relation defined in (1.6). "Having the same isotropy class" (or equivalentely the relation $\approx$) is coarser than the relation "being in the same orbit" (1.3) defined in the previous section. In fact, due to lemma 1.1.8, vectors of same G-orbit have the same isotropy class but the converse is not always true. Here is a counterexample.

Example 1.1.11. *Consider the usual action of* $\mathrm{SO}(2)$ *on* $\mathbb{R}^2$*. All vectors except* 0 *have conjugate symmetry groups but they are not in the same orbit.*

For an isotropy subgroup H of G (*i.e.* $H = G_{\boldsymbol{v}}$ for $\boldsymbol{v} \in V$), we gather the vectors having the same isotropy class in a set called the *isotropy stratum* with respect to H, denoted by $\Sigma_{[H]}$,

$$\Sigma_{[H]} := \{\boldsymbol{v} \in V; [G_{\boldsymbol{v}}] = [H]\}.$$

By lemma 1.1.10, we can observe that $\Sigma_{[H]} = V_{\boldsymbol{v}}^{\approx}$ (1.7) for the vectors $\boldsymbol{v} \in V$ such that $G_{\boldsymbol{v}} = H$. In other words, the isotropy stratum $\Sigma_{[H]}$ consists of the vectors $\boldsymbol{v}$ of V having isotropy group conjugated to H. Note that the isotropy strata are G-stable sets.

1.2 Linear representation of compact Lie groups

In this section, G denotes a compact Lie group and V a vector space. A *representation* of the group G on V is a continuous group morphism

$$\begin{aligned} \rho : \ & G \to \mathrm{GL}(V) \\ & g \mapsto \rho(g) \end{aligned}$$

where $\mathrm{GL}(V)$ denotes the group of linear automorphisms on V and for $\boldsymbol{v} \in V$, $\rho(g)\boldsymbol{v} = g \cdot \boldsymbol{v}$. A representation of a group G on a vector space V will be denoted by (V, G) or (V, ρ).

1.2.1 Reducibility

Definition 1.2.1. *A representation* (V, G) *is said to be* reducible *if there exists a non trivial subspace* W *of* V *(that is* $W \neq \{0\}$ *and* $W \neq V$*) that is* G*-stable. It is said to be* irreducible *if it is not reducible.*

Example 1.2.2. *The representation of the group* $\mathrm{SO}(n, \mathbb{R})$ *on* $\mathbb{R}^n$ *given by* $\rho(g)\boldsymbol{v} = g\boldsymbol{v}$*, if* $g \in \mathrm{SO}(n, \mathbb{R})$ *and* $\boldsymbol{v} \in \mathbb{R}^n$*, is irreducible.*

Definition 1.2.3. *A representation* (V, G) *is said to be* decomposable *if* V *can be decomposed into a direct sum of irreducible subspaces.*

Remark 1.2.4. *A decomposable representation is reducible but the converse is not always true. As a counterexample, consider the following representation of* $\mathbb{R}$ *on* $\mathbb{R}^2$

$$\rho(t)(x,y) = (x+ty, y),\ t \in \mathbb{R},\ (x,y) \in \mathbb{R}^2.$$

ρ *is reducible since* $E =< (1,0) >$ *is stable by* ρ*. However,* ρ *is not decomposable. Indeed, suppose that there exists a subspace* F *of* $\mathbb{R}^2$ *stable by* ρ *and such that* $E \oplus F = \mathbb{R}^2$*. Let* u *be a generating vector of* F $(\dim F = 1)$ *such that* $u = (u_1, 1)$ *with* $u_1 \in \mathbb{R}$ $(u_2 \neq 0$ *since* $u \notin E)$*. Since* F *is stable by* ρ *then,* $\forall t \in \mathbb{R}$*,* $\exists \lambda(t) \in \mathbb{R}$ *such that* $\rho(t)(u) = \lambda(t)u$*. In particular, for all* $t \in \mathbb{R}$*,* $\lambda(t) = 1$ *and then* u *is fixed by all* $\rho(t)$*,* $t \in \mathbb{R}$*, which leads to a contradiction.*

Definition 1.2.5. *A group* G *is said to be* linearly reductive *if every finite dimensional representation of* G *is decomposable.*

Lemma 1.2.6. *Every compact group is linearly reductive.*

Proof. Let $U \subset V$ be a G-stable subspace and $< \cdot, \cdot >$ be a G-invariant scalar product on V (which exists since G is compact; take for instance the scalar product defined, for $\boldsymbol{v}, \boldsymbol{w} \in V$, by $< \boldsymbol{v}, \boldsymbol{w} >:= \int_G (g \cdot \boldsymbol{v}, g \cdot \boldsymbol{w}) dg$ where $(\cdot, \cdot)$ is a scalar product on V and dg is the Haar measure (left and right Haar measure are the same since G is compact) on G (see [13, Chapter 0 section 3], [14, page 46])). Then $U^\perp = \{\boldsymbol{v} \in V;\ \forall u \in U,\ < \boldsymbol{v}, \boldsymbol{u} >= 0\}$ is a G-stable subspace of V such that $V = U \oplus U^\perp$. □

Remark 1.2.7. *When the group* G *is finite, the invariant scalar product defined in the previous proof becomes, if* $\boldsymbol{v}, \boldsymbol{w} \in V$*,* $< \boldsymbol{v}, \boldsymbol{w} >:= \dfrac{1}{|G|} \displaystyle\sum_{g \in G} (g \cdot \boldsymbol{v}, g \cdot \boldsymbol{w})$ *where* $|G|$ *denotes the number of elements of* G*.*

Example 1.2.8. *Consider the representation* ρ *of the group* $G = \mathrm{SO}(n)$ *on the space of real symmetric matrices* V *defined by*

$$\rho(g)A = gAg^{-1},\ \textit{for } g \in \mathrm{SO}(n) \textit{ and } A \in V.$$

ρ *is reducible since the subspace* U *generated by the identity matrix* I_n *is* G*-stable as well as its orthogonal* $U^\perp = \{A \in V;\ < A, \mathrm{I}_n >= 0\} = \{A \in V;\ \mathrm{tr}(A) = 0\}$ *(where* $< \cdot, \cdot >$ *is defined by, for* $A, B \in V$*,* $< A, B >= \mathrm{tr}(AB^T)$*). Moreover,* ρ *is decomposable since* V *can be decomposed in* $V = U \oplus U^\perp$ *where the representation of* G *on* $U^\perp$ *is irreducible. Indeed, since every symmetric matrix is diagonalisable in an orthonormal basis then each* G*-orbit intersect the subspace* D *of diagonal matrices. Since* D *is stable under the action of the permutation group* $\mathcal{S}_n$ *then the representation of* G *on* $U^\perp$ *is determined by the representation of* $\mathcal{S}_n$ *on* $D \cap U^\perp$ *which is irreducible.*

1.2.2 Isotropic stratification

As G is a compact group, a partial order relation can be defined on the set of the conjugacy classes of closed subgroups of G:

Theorem 1.2.9. *The relation on the set of conjugacy classes of closed subgroups of a compact group G defined by*

$$[H_1] \preceq [H_2] \text{ if } H_1 \text{ is conjugate to a subgroup of } H_2 \tag{1.9}$$

is a partial order relation.
To prove the anti-symmetricity of the relation (1.9), we make use of the following result:

Lemma 1.2.10. *[13, proposition 1.9] Let G be a compact group and H be a closed subgroup of G. If $H \subset gHg^{-1}$ for $g \in G$ then $H = gHg^{-1}$.*

Proof. Let $g \in G$ such that $H \subset gHg^{-1}$ then $\forall n \geq 1$, $gHg^{-1} \subset g^n H g^{-n}$. Let $h \in H$ then there exists $h_n \in H$ such that $ghg^{-1} = g^n h_n g^{-n}$. Since G is compact, for all $n \in \mathbb{N}$ there exists $k \in \mathbb{N}$ and $g' \in G$ such that the subsequence $(g^{n_k})_{n_k \in \mathbb{N}}$ of $(g^n)_{n \in \mathbb{N}}$ converges to g'. Set $m_k = n_{k+1} - n_k$, then we have $ghg^{-1} = g^{m_k} h_{m_k} g^{-m_k} \to h_{m_k}$. Since G is compact, there exists $r \in \mathbb{N}$ and $h' \in H$ such that the subsequence $(h_{m_{k_r}})_{m_{k_r} \in \mathbb{N}}$ of $(h_{m_k})_{m_k \in \mathbb{N}}$ converges to h'. It follows that $gHg^{-1} \subset H$ and hence the equality. □

proof of theorem 1.2.9. The reflexivity and the transitivity of $\preceq$ are straightforward. As for the anti-symmetricity, we use lemma 1.2.10: let H_1 and H_2 be two closed subgroups of G such that $[H_1] \preceq [H_2]$ and $[H_2] \preceq [H_1]$, then there exist $g_1, g_2 \in G$ such that $H_1 \subset g_1 H_2 g_1^{-1}$ and $H_2 \subset g_2 H_1 g_2^{-1}$. We have, on one hand,

$$H_1 \subset g_1 H_2 g_1^{-1} \subset g_1 g_2 H_1 (g_1 g_2)^{-1} \implies H_1 = (g_1 g_2) H_1 (g_1 g_2)^{-1},$$

and on the other hand

$$H_2 \subset g_2 H_1 g_2^{-1} \implies g_1 H_2 g_1^{-1} \subset (g_1 g_2) H_1 (g_1 g_2)^{-1} = H_1 \subset g_1 H_2 g_1^{-1}.$$

Hence, we deduce the result. □

The notions of orbit space, isotropy groups and isotropy classes, defined in section 1.1, extends naturally to the linear representations of a compact group. For an action of a finite group on a finite set, there exists a finite number of G-orbits. An interesting question arises here about the number of isotropy classes for a finite dimensional group representation.

Theorem 1.2.11. *Let G be a compact Lie group acting on a vector space V. Then there exists a finite number of isotropy classes.*

The finiteness of isotropy classes for a continuous action of a compact Lie group on a compact manifold was initially conjectured by Montgomery and solved by Mostow in [81] using the result of Floyd [36]. However, it is much easier in the case of a differentiable action (see [108, Theorem 5.11]). This implies the finiteness of isotropy classes for a linear representation of a compact Lie group : we can see it by extending a representation on V to an action on the projective compactification $\mathbb{P}(V \oplus \mathbb{R})$, or on the sphere $S(V)$ if we take an invariant inner product.

For a compact Lie group representation (V, ρ), the partition of V into (nonempty) isotropy strata

$$V = \Sigma_{[H_0]} \cup \cdots \cup \Sigma_{[H_n]}$$

is called its *isotropy stratification* or *orbit type stratification* with respect to the representation (V, ρ).

1.2.3 Principal isotropy stratum

To understand the geometry of conjugacy classes, a very useful notion is the notion of *slice*.

Definition 1.2.12. *For any $\boldsymbol{v}$ in V, a local slice of the G-action at v is a local submanifold $S \subset V$ passing through $\boldsymbol{v}$ such that:*

- *S is transverse to the orbit $G \cdot \boldsymbol{v}$ (i.e. $\forall p \in S \cap G \cdot \boldsymbol{v},\ T_pS \oplus T_p(G \cdot \boldsymbol{v}) = T_pV$).*
- *S is stable under $G_{\boldsymbol{v}}$.*
- *If s_1, s_2 are two points in S and if there exists g in G with $g \cdot s_1 = s_2$, then g belongs to $G_{\boldsymbol{v}}$. In particular, $G_s \subset G_{\boldsymbol{v}}$ for each point $s \in S$.*
- *$G \cdot S$ is an open neighborhood of the orbit $G \cdot \boldsymbol{v}$.*

Slices exist in general for proper smooth actions of Lie groups on manifolds (see [30, Theorem 2.3.1] for the precise hypothesis on the actions), and in particular for actions of compact Lie groups. However, for linear representations of compact Lie groups, it is possible to produce slices easily (see lemma B.3 of appendix B of chapter 2). The existence of slices has the following corollary.

Corollary 1.2.13. *Let $\boldsymbol{v}$ in V. Then there exists a neighborhood U of $\boldsymbol{v}$ such that for all $\boldsymbol{w}$ in U, $[G_{\boldsymbol{w}}] \preceq [G_{\boldsymbol{v}}]$.*

Proof. Let S be a slice at $\boldsymbol{v}$. If $\boldsymbol{w} \in G.S$ then $\boldsymbol{w}$ is in the orbit of a point $\boldsymbol{w}'$ in S. It follows that $G_{\boldsymbol{w}'} \subset G_{\boldsymbol{v}}$, so $[G_{\boldsymbol{w}}] = [G_{\boldsymbol{w}'}] \preceq [G_{\boldsymbol{v}}]$. □

Due to the existence of a partial order on conjugacy classes, points with locally minimal isotropy can be defined:

Definition 1.2.14. *A vector $\boldsymbol{v} \in V$ (or its orbit) is called* principal *if there exists a neighborhood U of $\boldsymbol{v}$ such that for all $\boldsymbol{w}$ in U, $[G_{\boldsymbol{w}}] = [G_{\boldsymbol{v}}]$. Equivalently, $\boldsymbol{v}$ is principal if it has locally minimal isotropy.*

Remark 1.2.15. *The set of principal points is open by definition.*

Let us denote by π the canonical projection from V to V/G. The principal orbit type theorem can be stated (in the case of linear representations) as follows (see [13, Theorem 3.1], [1, section VI], [30, Theorem 2.8.5]).

Theorem 1.2.16 (Principal orbit type theorem)**.** *For any open subset Ω of V such that $\pi(\Omega)$ is connected, the set U_Ω of principal points in Ω is open, dense in Ω and U_Ω/G is connected.*

A proof of this theorem is provided in appendix B of chapter 2.
It follows from the connectivity of U_Ω/G that there is a unique isotropy stratum $\Sigma_{[H_0]}$ which is minimal. This isotropy class $[H_0]$ is called the *principal stratum*. We can conclude that the principal orbit type $[H_0]$ is the *smallest* isotropy class.

Example 1.2.17. *Consider, for instance, the representation of the rotation group $G = \mathrm{SO}(3)$ on the space of symmetric 3×3 matrices. Then there are exactly three orbit types*

$$[\mathbb{D}_2] \preceq [\mathrm{O}(2)] \preceq [\mathrm{SO}(3)]$$

where $[\mathbb{D}_2]$ is the principal stratum.

1.2.4 Closed isotropy stratum

Let H be subgroup of G. We define the *fixed point set* V^H, which is a vector subspace of V, by

$$V^H := \{\boldsymbol{v} \in V \mid h \cdot \boldsymbol{v} = \boldsymbol{v} \text{ for all } h \in H\},$$

and the *isotropy stratum* $\Sigma_{[H]}$ by

$$\Sigma_{[H]} := \{\boldsymbol{v} \in V;\ [G_{\boldsymbol{v}}] = [H]\}.$$

We define the open fixed locus $\overset{\circ}{V}{}^H$ which is a subset of V^H:

$$\overset{\circ}{V}{}^H := \{\boldsymbol{v} \in V;\ G_{\boldsymbol{v}} = H\} \subset V^H.$$

This definition makes the stratum $\Sigma_{[H]}$ the orbit of $\overset{\circ}{V}{}^H$.

Remark 1.2.18. *If H_1 and H_2 are two subgroups of G such that $H_1 \subset H_2$ then $V^{H_2} \subset V^{H_1}$. Indeed, if $\boldsymbol{v} \in V^{H_2}$ then for all $h \in H_2$, $h \cdot \boldsymbol{v} = \boldsymbol{v}$. In particular, for all $h \in H_1$, $h \cdot \boldsymbol{v} = \boldsymbol{v}$. However, it may happen that $V^{H_1} = V^{H_2}$ for $H_1 \neq H_2$.*

As a consequence of the order relation defined on the conjugacy classes in 1.2.9, we define *closed isotropy stratum* with respect to an isotropy subgroup H to be the set consisting of vectors having *at least the symmetry* of H. The closed isotropy stratum with respect to H is denoted by $\overline{\Sigma}_{[H]}$ and given by

$$\overline{\Sigma}_{[H]} = \left\{\boldsymbol{v} \in V;\ G_{\boldsymbol{v}} \supset gHg^{-1} \text{ for some } g \in G\right\} = \bigcup_{[H] \preceq [K]} \Sigma_{[K]}.$$

The closed stratum is the orbit of V^H.

Remark 1.2.19.

- *The terminology we use above is not totally standard, but in literature the terminology varies according to the authors (for instance, what we call stratum is called orbit bundle in [108]).*

- *The fixed locus V^H is defined for arbitrary closed subgroups of G (not only isotropy subgroups) but we will generally avoid to do so.*
- *The terminology "closed stratum" and the corresponding notation will be justified by Corollary 1.2.22. The same holds for the open fixed locus.*
- *The partial order relation on isotropy classes induces a (reverse) partial order relation on the strata: if H_1, H_2 are two isotropy subgroups of G,*

$$[H_1] \preceq [H_2] \iff \Sigma_{[H_2]} \preceq \Sigma_{[H_1]}$$

Proposition 1.2.20. *Let H be an isotropy subgroup. Then $\overset{\circ}{V}{}^H$ is open and dense in V^H, more precisely it contains an open dense subset of V^H.*

Proof. Let $\boldsymbol{x}$ be in $\overset{\circ}{V}{}^H$. Then thanks to Corollary 1.2.13 there exists a neighborhood U of $\boldsymbol{x}$ such that for $\boldsymbol{y}$ in U, $[G_{\boldsymbol{y}}] \preceq [H]$. If $\boldsymbol{y}$ in $U \cap V^H$, $[H] \preceq [G_{\boldsymbol{y}}] \preceq [H]$ so $[G_{\boldsymbol{y}}] = [H]$. This means that $H \subset G_{\boldsymbol{y}} = gHg^{-1}$ for some g in G so $G_{\boldsymbol{y}} = H$ by lemma 1.2.10. This proves that $\overset{\circ}{V}{}^H$ is open. The second part is difficult and will be proven later (see Corollary 3.17 of chapter 2). □

Remark 1.2.21. *For polynomial actions, an open dense subset is also a Zariski open [1] subset.*

Corollary 1.2.22. *$\overline{\Sigma}_{[H]}$ is the closure of $\Sigma_{[H]}$.*

Proof. First we prove that $\overline{\Sigma}_{[H]}$ is closed. If $(\boldsymbol{v}_n)_{n\in\mathbb{N}}$ is a sequence in $\overline{\Sigma}_{[H]}$ that converges to a vector $\boldsymbol{v} \in V$ then, for all $n \in \mathbb{N}$, there exists an element g_n in G such that, $\forall n \in \mathbb{N}$, $g_n H g_n^{-1} \subset G_{\boldsymbol{v}_n}$. Extracting a subsequence, we can assume that $(g_n)_{n\in\mathbb{N}}$ converges to an element g in G. Then $gHg^{-1} \subset G_{\boldsymbol{v}}$ so that $\boldsymbol{v}$ belongs to $\overline{\Sigma}_{[H]}$. Now, let $\boldsymbol{v}$ be in $\overline{\Sigma}_{[H]}$. By definition, there exists g in G such that $g^{-1} \cdot \boldsymbol{v}$ belongs to V^H. Thanks to proposition 1.2.20, $g^{-1} \cdot \boldsymbol{v}$ is the limit of a sequence of elements in $\overset{\circ}{V}{}^H$. □

1.2.5 Action of the monodromy group

Let G be a compact Lie group acting linearly on V.

If H is a subgroup of G, We define the *normalizer* $N(H)$ of H by

$$N(H) = \left\{ g \in G \mid gHg^{-1} = H \right\}. \tag{1.10}$$

Remark 1.2.23. *Note that $N(H)$ is the maximal subgroup of G in which H is a normal subgroup. Indeed, $N(H)$ is the isotropy subgroup of H for the action of the group G on the set of all subgroups of G, defined by*

$$g \cdot K = gKg^{-1}, \qquad \text{if } g \in G \text{ and } K \text{ is a subgroup of } G.$$

We have the following result (see [2], [43]) :

[1] A Zariski open set is the complement set of zeros of a finite number of polynomials

Lemma 1.2.24. *For each closed subgroup H of G, V^H is $N(H)$-stable. Moreover, if $H = G_{\boldsymbol{v}_0}$ is the* isotropy group *of some vector $\boldsymbol{v}_0 \in V$, then $N(H) = \{g \in G; \mid g \cdot V^H \subset V^H\}$.*

Proof. Let $\boldsymbol{v}$ in V^H. For any g in $N(H)$ and any h in H, $h \cdot (g \cdot \boldsymbol{v}) = g \cdot (g^{-1}hg) \cdot \boldsymbol{v} = g \cdot \boldsymbol{v}$ (since $g \in N(H)$). If moreover $H = G_{\boldsymbol{v}_0}$ and $g \in G$ is such that $g \cdot V^H \subset V^H$, then $g \cdot \boldsymbol{v}_0$ is in V^H but $G_{g \cdot \boldsymbol{v}_0} = gG_{\boldsymbol{v}_0}g^{-1}$ and thus $H \subset gHg^{-1}$. By lemma 1.2.10, since H is compact, g belongs to $N(H)$. □

The action of G on V induces an action of $N(H)$ on V^H and we can therefore reduce (locally) the problem of describing the orbit space of V/G by the orbit space of $V^H/N(H)$.

Lemma 1.2.25. *Given an isotropy subgroup H and a vector $\boldsymbol{v} \in V^H$ then, for all $\boldsymbol{w} \in \Sigma_{[H]} \cap V^H$,*

$$\boldsymbol{w} \text{ belongs to the } G\text{-orbit of } \boldsymbol{v} \text{ in } V \iff \boldsymbol{w} \text{ belongs to the } N(H)\text{-orbit of } \boldsymbol{v} \text{ in } V^H.$$

Proof. Let $\boldsymbol{v} \in V^H$ and $\boldsymbol{w} \in \Sigma_{[H]} \cap V^H$ such that $\boldsymbol{w} \in G \cdot \boldsymbol{v}$ then there exists $g \in G$ such that $\boldsymbol{w} = g \cdot \boldsymbol{v}$. Since $\boldsymbol{w} \in \Sigma_{[H]} \cap V^H$ and by lemma 1.2.10, $H = G_{\boldsymbol{w}}$. Hence, $H = gG_{\boldsymbol{v}}g^{-1}$ and we have $H \subset G_{\boldsymbol{v}}$ (since $\boldsymbol{v} \in V^H$). Applying one more time lemma 1.2.10, we deduce that $G_{\boldsymbol{v}} = gG_{\boldsymbol{v}}g^{-1} = H$. Therefore, $g \in N(H)$ and hence $\boldsymbol{w} \in N(H) \cdot \boldsymbol{v}$. The converse is straightforward. □

The representation $\rho_{N(H)}$ of $N(H)$ on V^H is not faithful. When H is an isotropy group, its kernel $\left(\ker(\rho_{N(H)}) = \{g \in N(H) \mid \forall \boldsymbol{v} \in V^H,\ \rho_{N(H)}(g)\boldsymbol{v} = \boldsymbol{v}\}\right)$ is exactly H therefore, by applying lemma 1.1.6, we get the following *faithful* linear representation

$$\rho_\Gamma : \Gamma \longrightarrow \mathrm{GL}(V^H) \text{ where } \Gamma := N(H)/H.$$

When Γ is finite, each G-orbit intersects V^H at most in a finite number of points, in this case, V^H is called a *linear slice* and Γ will be its *monodromy group*. The cardinal of the monodromy group determine the number of points in the intersection of each G-orbit of a point of $\mathring{V}^H$ and V^H. In particular, when Γ is the trivial group then each G-orbit meets V^H in at most one point.

1.3 Algebras of invariants and covariants

1.3.1 Action of a group on the algebra of invariants

Let $\mathbb{K}$ be the field $\mathbb{R}$ or $\mathbb{C}$ and consider the polynomial algebra $\mathbb{K}[V]$ consisting of all polynomial functions on V with coefficients in $\mathbb{K}$. The linear action of the group G on the vector space V extends naturally to $\mathbb{K}[V]$ setting as follows

$$(g \cdot P)(\boldsymbol{v}) := P(g^{-1} \cdot \boldsymbol{v})$$

if $P \in \mathbb{K}[V]$ and $\boldsymbol{v} \in V$. We define the set of all polynomial functions on V that are *invariant* under the action of G, denoted by $\mathbb{K}[V]^G$,

$$\mathbb{K}[V]^G = \{P \in \mathbb{K}[V] \mid \forall g \in G,\ g \cdot P = P\}.$$

$\mathbb{K}[V]^G$ is a subalgebra over $\mathbb{K}$ of the algebra $\mathbb{K}[V]$ called the *invariant algebra*.

1.3.2 Integrity basis

The following result is due to Hilbert ([50], see also chapter 2 subsection 1.3.1).

Theorem 1.3.1. *For every linear algebraic reductive group, the invariant algebra $\mathbb{K}[V]^G$ is finitely generated.*

This means that there exists a finite set of invariant polynomials $I_1, \ldots, I_N$ which generate the invariant algebra $\mathbb{K}[V]^G$:

$$\mathbb{K}[V]^G = \mathbb{K}[I_1, \ldots, I_N].$$

Such a family $I_1, \ldots, I_N$ is called an *integrity basis*.

The actual determination of an integrity basis remains a very active field of research. Below, we give some examples.

Example 1.3.2. *1. The case of the natural representation $(\mathrm{SO}(3), \mathbb{R}^3)$ for which an integrity basis is simply given by the squared norm:*

$$\mathbb{R}[\mathbb{R}^3]^{\mathrm{SO}(3)} = \mathbb{R}[I], \quad I(\boldsymbol{v}) := \|\boldsymbol{v}\|^2.$$

2. The standard representation $(\mathrm{SO}(3), \mathbb{S}_2(\mathbb{R}^3))$, where we have

$$\mathbb{R}[\mathbb{S}_2(\mathbb{R}^3)]^{\mathrm{SO}(3)} = \mathbb{R}[I_1, I_2, I_3], \quad I_k := \mathrm{tr}(\mathbf{a}^k), \ k = 1, 2, 3.$$

3. The case of standard representation of the group of permutations $\mathcal{S}_n$ on $\mathbb{R}^n$:

$$\mathbb{R}[\mathbb{R}^n]^{\mathcal{S}_n} = \mathbb{R}[\sigma_1, \ldots, \sigma_n]$$

where σ_i are the elementary symmetric functions

$$\sigma_1(\boldsymbol{x}) = x_1 + \ldots + x_n, \ \sigma_2(\boldsymbol{x}) = \Sigma_{i \neq j} x_i x_j, \ \ldots, \ \sigma_n(\boldsymbol{x}) = x_1 \ldots x_n, \quad \boldsymbol{x} = (x_1, ; \ldots, x_n) \in \mathbb{R}^n.$$

Definition 1.3.3. *A* minimal integrity basis *is an integrity basis such that none of its elements can be expressed as a polynomial of the others.*

Remark 1.3.4. *A minimal integrity basis is not unique, however, all of them have the same cardinal and the list of the degrees of the generators are the same (see for instance [44, section 5.1.1]).*

An important property of polynomial invariants for a real representation of a compact group (and thus of any integrity basis) is that they separate the orbits, which means that given two vectors $\boldsymbol{v}_1, \boldsymbol{v}_2 \in V$ belonging to different orbits, it is always possible to find a function $p \in \mathbb{R}[V]^G$ such that $p(v_1) \neq p(v_2)$ (see for instance [1, Appendix C]). In other words,

$$\forall p \in \mathbb{R}[V]^G, \ p(\boldsymbol{v}_1) = p(\boldsymbol{v}_2) \iff \boldsymbol{v}_1 = g \cdot \boldsymbol{v}_2 \text{ for some } g \in G.$$

Example 1.3.5. *For instance, two vectors* $\boldsymbol{v}$, $\boldsymbol{w} \in \mathbb{R}^2$ *are related by a rotation if and only if they have the same norms* $\|\boldsymbol{v}\|^2 = \|\boldsymbol{w}\|^2$.

Using this fact, the orbit space V/G can then be described as a semialgebraic subset of $\mathbb{R}^N$. Indeed, if $\{p_1, \ldots, p_N\}$ denotes a generating set for $\mathbb{R}[V]^G$, then the mapping

$$P : v \mapsto \big(p_1(v), p_2(v), \ldots, p_N(v)\big)$$

induces an homeomorphism between V/G and $P(V) \subset \mathbb{R}^N$ which is a semialgebraic subset of $\mathbb{R}^N$ (see [95]).

In the same way as is defined the algebra of polynomial invariants $K[V]^G$, one can define the *invariant field* $K(V)^G$ of *rational invariants*, which is a subfield of the field $K(V)$ of all rational functions on V. Note that this field is always finitely generated since it is contained in the finitely generated field $K(V)$ (see for instance [20, theorem 11.23]). Algorithms for constructing a generating set of rational invariants for the invariant field $K(V)^G$ exist and can be used to express any rational invariant in terms of the generators (see [51, 52]).

1.3.3 Covariant algebra

In [62], Kraft and Procesi have generalized the concept of invariants in the following way.

Definition 1.3.6. *Given two representations* $\mathbb{V}$ *and* $\mathbb{W}$ *of a group* G*, we define* $\mathrm{Pol}(\mathbb{V}, \mathbb{W})$ *to be the space of polynomial mappings* p *from* $\mathbb{V}$ *to* $\mathbb{W}$. $\mathrm{Pol}(\mathbb{V}, \mathbb{W})$ *is a vector space of* V *on which* G *acts linearly:*

$$\forall \boldsymbol{v} \in \mathbb{V}, \forall g \in G,\ g(\mathrm{p}(g \cdot \boldsymbol{v})) = g \cdot \mathrm{p}(\boldsymbol{v})$$

A polynomial covariant of $\mathbb{V}$ of type $\mathbb{W}$ *is a* G*-equivariant polynomial mapping* $\mathrm{p} : \mathbb{V} \to \mathbb{W}$*, which means that*

$$\forall \boldsymbol{v} \in \mathbb{V}, \forall g \in G,\ \mathrm{p}(g \cdot \boldsymbol{v}) = g \cdot \mathrm{p}(\boldsymbol{v}).$$

We denote by $\mathrm{Pol}(\mathbb{V}, \mathbb{W})^G$ the set of polynomial covariant of $\mathbb{V}$ of type $\mathbb{W}$.

The space $\mathrm{Pol}(\mathbb{V}, \mathbb{W})^G$ can be identified with the space $\mathrm{L}(\mathbb{W}^*, \mathbb{K}[\mathbb{V}])$ of all linear mapping from $\mathbb{W}^*$ into $\mathbb{K}[\mathbb{V}]$. Indeed, this correspondence comes from the identification of $\mathrm{Pol}(\mathbb{V}, \mathbb{W})^G$ with $\mathbb{K}[\mathbb{V}] \otimes \mathbb{W}$.

This algebraic structure of $\mathrm{Pol}(\mathbb{V}, \mathbb{W})^G$ will be then extended to create the covariant algebra (see also [94, Page 184] for a more general and abstract definition of this concept).

Definition 1.3.7. *Let* $\mathbb{V}, \mathbb{W}$ *be finite-dimensional representations of a group* G *and* $\mathbb{W}^*$ *the dual vector space of* $\mathbb{W}$*. The* covariant algebra of $\mathbb{V}$ of type $\mathbb{W}$*, noted* $\mathbf{Cov}(\mathbb{V}, \mathbb{W})$*, is defined as the invariant algebra*

$$\mathbb{K}[\mathbb{V} \oplus \mathbb{W}^*]^G.$$

Note that the covariant algebra $\mathbf{Cov}(\mathbb{V}, \mathbb{W})$ has a natural bi-graduation. It is the direct sum of the finite dimensional vector spaces $\mathbf{Cov}_{d,k}(\mathbb{V}, \mathbb{W})$ of bi-homogeneous polynomial $p(\boldsymbol{v}, \omega)$:

- of total degree d in $\boldsymbol{v} \in \mathbb{V}$, called the **degree** of the covariant,
- and, of total degree k in $\omega \in \mathbb{W}^*$, called the **order** of the covariant.

Furthermore, the subspace of covariants of order 0 is identical to the invariant algebra of $\mathbb{V}$.

Remark 1.3.8. *The vector space of polynomial covariants* $\mathrm{Pol}(\mathbb{V},\mathbb{W})^G$ *can thus be identified with*

$$\mathbf{Cov}_1(\mathbb{V},\mathbb{W}) = \bigoplus_{k=0}^{+\infty} \mathbf{Cov}_{k,1}(\mathbb{V},\mathbb{W}),$$

the vector space of first-order covariants.

Example 1.3.9. *When* $G = \mathrm{SO}(3)$ *and* $\mathbb{W}$ *is the Euclidean space* $\mathbb{R}^3$*, the covariant algebra of a finite-dimensional representation* $\mathbb{V}$ *is given by*

$$\mathbf{Cov}(\mathbb{V}) := \mathbb{R}[\mathbb{V} \oplus \mathbb{R}^3]^{\mathrm{SO}(3)}.$$

An element $\mathrm{p} \in \mathbf{Cov}(\mathbb{V})$ *is thus a polynomial which can be written as*

$$\mathrm{p}(\boldsymbol{v},\boldsymbol{x}) = \sum_{i,j,k} p_{ijk}(\boldsymbol{v}) x^i y^j z^k,$$

where each coefficient $p_{ijk}(\boldsymbol{v})$ *is a polynomial function of* $\boldsymbol{v}$*, and such that*

$$\mathrm{p}(g \cdot \boldsymbol{v}, \boldsymbol{x}) = \mathrm{p}(\boldsymbol{v}, g^{-1} \cdot \boldsymbol{x}),$$

for all $\boldsymbol{v} \in \mathbb{V}$*,* $\boldsymbol{x} \in \mathbb{R}^3$ *and* $g \in \mathrm{SO}(3)$*.*

Like the invariant algebra, the covariant algebra of a finite-dimensional representation of a compact group is finitely generated.

Theorem 1.3.10 (Hilbert's Theorem [50])**.** *The covariant algebra* $\mathbf{Cov}(\mathbb{V})$ *is finitely generated, i.e. there exists a finite set* $\mathcal{B} := \{\mathrm{p}_1, \ldots, \mathrm{p}_s\}$ *in* $\mathbf{Cov}(\mathbb{V})$ *such that*

$$\mathbf{Cov}(\mathbb{V}) = \mathbb{R}[\mathrm{p}_1, \ldots, \mathrm{p}_s].$$

Chapter 2

Rationality of normal forms of isotropy strata

This chapter is an ArXiv preprint in which we study the isotropy stratification of a linear representation V of a compact Lie group G. We achieve two important results. First, we prove that for each isotropy subgroup H, every rational invariant of the induced representation $(V^H, N(H))$ can be obtained as the restriction of a global invariant of (V, G), where $N(H)$ is the normalizer of H and V^H is the fixed point set of H. Second, we prove that the closed isotropy strata are real algebraic sets being an irreducible component of the real locus of an algebraic complex variety. The proof appeals to theorems and results on the geometry of orbits that hold only for algebraically closed field. Since we work with real representations of real groups, a detailed theory on the complexification of a real linear representation of a compact Lie group is fully provided in this chapter. Finally, in the appendix B, we give a proof for the principal orbit theorem in the linear case using linear slices.

RATIONALITY OF NORMAL FORMS OF ISOTROPY STRATA OF A REPRESENTATION OF A COMPACT LIE GROUP

P. AZZI, R. DESMORAT, J. GRIVAUX, AND B. KOLEV

Abstract. In this article we study the isotropy stratification of a linear representation V of a compact Lie group G. We prove that the closed isotropy strata are real algebraic manifolds and that for each isotropy subgroup H, every rational invariant of the induced representation $(V^H, N(H))$ can be obtained as the restriction of a global invariant of (V, G), where $N(H)$ is the normalizer of H and V^H is the fixed point set of H.

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1. Introduction

It was observed in [2], on an example from solid mechanics, that the coefficients of the normal form for some orbit types (also called *isotropy classes* or *symmetry classes* in mechanics) of a tensorial representation $(V, \mathrm{SO}(3))$ could be expressed rationally using some polynomial invariants of $(V, \mathrm{SO}(3))$. Let us start by giving an example of what we mean by this assertion. Consider the natural representation of the rotation group $\mathrm{SO}(3, \mathbb{R})$ on the vector space $\mathbb{H}^2(\mathbb{R}^3)$ of traceless symmetric 3×3 matrices with real coefficients

$$\rho(g)A = gAg^{-1}, \qquad A \in \mathbb{H}^2(\mathbb{R}^3), \quad g \in \mathrm{SO}(3, \mathbb{R}).$$

For this representation, there are exactly three orbit types corresponding to the symmetry groups $\mathbb{D}_2$ (three distinct eigenvalues, generic case), $\mathrm{O}(2)$ (two distinct eigenvalues) and $\mathrm{SO}(3)$ (only one eigenvalue). A normal form for the second orbit type represented by the symmetry group $\mathrm{O}(2)$ is provided by the linear subspace

$$V^{\mathrm{O}(2)} = \left\{A \in \mathbb{H}^2(\mathbb{R}^3);\ gAg^{-1} = A, \quad \forall g \in \mathrm{O}(2)\right\} = \left\{\mathrm{diag}(-\lambda, -\lambda, 2\lambda);\ \lambda \in \mathbb{R}\right\}.$$

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Then, on the dense open subset $\lambda \neq 0$ of $(\mathbb{H}^2(\mathbb{R}^3))^{\mathrm{O}(2)}$, one has $\lambda = \dfrac{I_3}{I_2}$, where $I_2 = \operatorname{tr} A^2$ and $I_3 = \operatorname{tr} A^3$ are a generating set of the invariant algebra

$$\mathbb{R}[\mathbb{H}^2(\mathbb{R}^3)]^{\mathrm{SO}(3,\mathbb{R})}.$$

More generally, consider a linear representation $\rho\colon G \to \mathrm{GL}(V)$ of a compact Lie group G on a real vector space V. Given an orbit type represented by a symmetry group $H \subset G$, each orbit of this type intersects the fix point set V^H, which may be considered as a normal form for these orbits. The normalizer $N(H)$ of H in G stabilizes the linear subspace V^H and ρ induces a faithful representation of $N(H)/H$ on V^H. It was conjectured, after the observations in [2], that every polynomial invariant of this representation is indeed the restriction on V^H of a rational invariant of the initial representation ρ of G. In a subsequent paper [33], it was moreover conjectured that the closed strata of any real linear representation V of a compact Lie group were moreover real algebraic subset of V. In this paper, we will prove the following theorem:

Theorem 1.1. *Let $\rho\colon G \to \mathrm{GL}(V)$ be a linear representation of compact Lie group G on a real vector space V, let H be an isotropy group of ρ, let $N(H)$ be the normalizer of H in G, and let V^H be the fixed locus of H.*

(1) *Every rational invariant of the induced representation $(V^H, N(H))$ is the restriction of an invariant of (V, G) which is rationally defined on V^H. In other words, the restriction map $\mathbb{R}[V] \to \mathbb{R}[V^H]$ induces a morphism*

$$S : \mathbb{R}(V)^G \dashrightarrow \mathbb{R}(V^H)^{N(H)},$$

which is surjective when restricted to its domain of definition.

(2) *The closed stratum $\overline{\Sigma}_{[H]}$ is a closed real algebraic subset of V.*

Related results can be found in the literature but under different hypotheses. In almost all papers, the problem is considered in the complex case and for generic orbit types. The most classical result fitting in this framework is Chevalley's restriction theorem that corresponds to a connected semisimple complex Lie group acting by the adjoint action on its Lie algebra $\mathfrak{g}$. More generally, Luna in [29] and then Luna and Richardson in [30, theorem 4.2] proved that, for a linear action of a reductive group G on an affine variety V (hence in particular for a vector space), the restriction map $K[V] \to K[V^H]$ maps $K[V]^G$ isomorphically onto $K[V^H]^\Gamma$ when K is an algebraically closed field, and H is the generic isotropy, and $\Gamma = N(H)/H$ (see also [29],[36]). Further results can be found in [15, 21, 31, 34] where the same isomorphism is proved on the fields of invariants of (V, G) and $(V(H), N(H))$ (that is $K(V)^G \simeq K(V^H)^\Gamma$) under the hypothesis that K is an algebraically closed field. To illustrate our theorem we provide below some explicit examples.

Example 1.2. We start with the real version of Chevalley's restriction theorem. If G is a connected compact Lie group, all maximal tori are conjugate (see [8, Chap. IV Thm 1.6]) and they are maximal abelian subgroups. Let r denote the rank of G, which is the dimension of any maximal torus T in G. Recall that an element x of $\mathfrak{g}$ is *regular* if the closure of the 1-parameter subgroup of G generated by x is a maximal torus in G. Regular points form a dense open subset $\mathfrak{g}^{\mathrm{reg}}$ of $\mathfrak{g}$, and for any x in $\mathfrak{g}^{\mathrm{reg}}$, G_x is the centralizer of the maximal torus of G containing the 1-parameter subgroup generated by x, which is the torus itself. Hence, if T is a maximal torus, if $W = N(T)/T$ is the corresponding Weil group, and if $\mathfrak{t}$ is the Lie algebra of T, there is an isomorphism $\mathbb{R}[V]^G \simeq \mathbb{R}[\mathfrak{t}]^W$ (see [8, Chap. VI Prop. 2.1]). Our result implies a weak form of this statement, namely the same isomorphism at the level of fields of invariants.

Example 1.3. For the standard representation of the symmetric group $\mathfrak{S}_3$ on $V = \mathbb{R}^3$, there are three isotropy classes $[\mathbb{1}]$, $[\mathfrak{S}_2]$, $[\mathfrak{S}_3]$. The invariant algebra $\mathbb{R}[\mathbb{R}^3]^{\mathfrak{S}_3}$ is generated by the three elementary symmetric functions σ_1, σ_2 and σ_3. The fixed point set $V^{\mathfrak{S}_2}$ is the plane $x = y$ and

$N(\mathfrak{S}_2) = \mathfrak{S}_2$. Hence, $\mathbb{R}[V^{\mathfrak{S}_2}]^{N(\mathfrak{S}_2)} = \mathbb{R}[x, y]$ and we have

$$x = \frac{\sigma_1\sigma_2 - 9\sigma_3}{2\sigma_1^2 - 6\sigma_2} \quad \text{and} \quad z = \frac{\sigma_1^3 - 4\sigma_1\sigma_2 + 9\sigma_3}{\sigma_1^2 - 3\sigma_2}.$$

Example 1.4. Here, we provide an example where $N(H)/H$ is not trivial. We consider the representation of the rotation group $\mathrm{SO}(3, \mathbb{R})$ on the vector space $V = \mathbb{H}^4(\mathbb{R}^3)$ of harmonic symmetric tensors of order 4 (or homogeneous harmonic polynomials in three variables of degree four). It is known, see [14, 16], that there are eight orbit types, and among them the symmetry class $[\mathbb{D}_2]$, where $\mathbb{D}_2$ is the dihedral group of order 2. The invariant algebra $\mathbb{R}[\mathbb{H}^4(\mathbb{R}^3)]^{\mathrm{SO}(3,\mathbb{R})}$ is generated by 9 polynomials J_k which have been obtained in [3] (see also [2]). The normalizer $N(\mathbb{D}_2)$ is the octahedral group $\mathbb{O}$ and $\Gamma = N(\mathbb{D}_2)/\mathbb{D}_2 \simeq \mathfrak{S}_3$. The fixed point set $V^{\mathbb{D}_2}$ is the three-dimensional vector space spanned by the harmonic polynomials

$$\begin{cases} p_1 = -z^4 + 6y^2z^2 - y^4, \\ p_2 = -z^4 + 6x^2z^2 - x^4, \\ p_3 = -y^4 + 6x^2y^2 - x^4. \end{cases}$$

In this basis, the action of the monodromy group $\Gamma \simeq \mathfrak{S}_3$ is just the standard action of the permutation group $\mathfrak{S}_3$ on the triple $(\lambda_1, \lambda_2, \lambda_3)$ and the invariant algebra $\mathbb{R}[V^{\mathbb{D}_2}]^{\mathfrak{S}_3}$ is generated by the elementary symmetric polynomials $(\sigma_1, \sigma_2, \sigma_3)$ in the λ_i. It was shown in [2] that σ_1, σ_2 and σ_3 can be expressed rationally in terms of the J_k by

$$\begin{cases} \sigma_1 = -\dfrac{9\,\left(3\,J_7 - 3\,J_2\,J_5 + 3\,J_3\,J_4 - {J_2}^2\,J_3\right)}{2\,\left(6\,J_6 - 9\,J_2\,J_4 - 20\,{J_3}^2 + 3\,{J_2}^3\right)}, \\ \sigma_2 = \dfrac{4}{7}\,{\sigma_1}^2 - \dfrac{1}{14}\,J_2, \\ \sigma_3 = \dfrac{1}{24}\,J_3 + \dfrac{1}{7}\,{\sigma_1}^3 - \dfrac{1}{56}\,\sigma_1\,J_2. \end{cases}$$

Outline. The article is organized as follows. In section 2, we recall basic material on representations of compact Lie groups and invariant theory. In section 3, we recall an explicit linear model for the complexification of a compact Lie group and provide several useful results on the complexification of a real continuous representation of a compact Lie groups. Besides, we prove one key technical tool, namely that for compact group, normalizers commute with complexification. The section 4 is devoted to the proof of theorem 1.1. In addition, two appendices are provided. In Appendix A, we recall some results about Lie groups, real analytic functions, and totally real manifolds. Finally, in Appendix B, we provide for the reader's convenience a proof of the Principal Orbit Theorem in the linear case.

2. Preliminaries

2.1. **Linear representations of compact Lie groups.** Let G be a compact (real) Lie group and let $\rho : G \to \mathrm{GL}(V)$ be a continuous linear representation of G on a finite dimensional vector space V. It is well-known that ρ is real-analytic (see corollary A.2). In particular, we will be able to apply all the tools of differential topology concerning smooth action of Lie groups on manifolds. We write $g \cdot v := \rho(g)v$ to lighten the notation.

For any vector v in V, we denote by $G \cdot v$ its orbit under G. The quotient set V/G of V under the action of G is the orbit space of V.

The *isotropy subgroup* (or *symmetry group*) of a vector v in V is defined by

$$G_v := \{g \in G;\ g \cdot v = v\}.$$

It is a closed subgroup of G, hence a Lie subgroup of G. The orbit $G \cdot v$ is a smooth compact submanifold of V, which is diffeomorphic to the homogeneous space G/G_v.

Two vectors in the same orbit have conjugate symmetry groups. Indeed,

$$\forall v \in V,\ \forall g \in G, \quad G_{g\cdot v} = g\ G_v\ g^{-1}.$$

Of course, the converse is false but we say that v_1 and v_2 are in the same *isotropy class* (or have the same *orbit type* in the terminology of [1]) if their symmetry groups are *conjugate* in G, that is if there exists $g \in G$ such that

$$G_{v_2} = g\, G_{v_1} g^{-1}.$$

Given a closed subgroup H of G, we say that the conjugacy class $[H]$ of H in G is an *isotropy class* (or an *orbit type*) if there exists a vector v such that $[H] = [G_v]$.

The finiteness of isotropy classes for a continuous action of a compact Lie group on a compact manifold was initially conjectured by Montgomery and solved in [13, 32] (in the case of a smooth action it is way more easy, see also [4, Chapter VII] and [38, Theorem 5.11]). This implies the finiteness of isotropy classes for a linear representation of a compact Lie group: we can see it by extending a representation on V to an action on the projective compactification $\mathbb{P}(V \oplus \mathbb{R})$, or on the sphere $S(V)$ if we take an invariant inner product.

Given a compact Lie group G, the inclusion relation on the set of closed subgroups induces a partial order on the set of their conjugacy classes [7, 1], called by some authors *containment relation* [9]. It is defined as follows:

$$[H_1] \preceq [H_2], \qquad \text{if } H_1 \text{ is conjugate to a subgroup of } H_2.$$

To understand the geometry of conjugacy classes, a very useful notion is that of a *slice*. We recall here the general definition, but in our setting not all properties are necessary (see 2.2).

Definition 2.1. For any v in V, a local slice of the G-action at v is an embedded disc $S \subset V$ passing through v such that:

- S is transverse to the orbit $G \cdot v$.
- S is stable under G_v.
- If s_1, s_2 are two points in S and there exists g in G with $g \cdot s_1 = s_2$, then g belongs to G_v. In particular, $G_s \subset G_v$ for each point $s \in S$.
- $G \cdot S$ is an open neighborhood of the orbit $G \cdot v$.

Remark 2.2. We have furthermore the following properties.

- Given a slice S, the open G-stable neighborhood $G \cdot S$ is diffeomorphic to the quotient $G \times_{G_v} S$, and after linearizing the action of G_v on S, $G \cdot S$ is locally diffeomorphic to $G \times_{G_v} N_v$ where N_v is the normal space of the orbit at v (viewed as a representation of the isotropy group G_v).
- Slices exist in general for proper actions of Lie groups on manifolds [10, Theorem 2.3.1], and in particular for actions of compact Lie groups. However, for linear representations of compact Lie groups, it is possible to produce slices easily (see lemma B.3 below).
- In our settings, where G is compact, the two last properties are automatic (of course up to shrinking S) as soon as the two first ones are granted.
- The last property can be made slightly stronger: up to shrinking S, we can even assume that the orbit map from $G \times S$ to V is a submersion, in particular it is an open map.

The existence of slices has the following corollary.

Corollary 2.3. *Let v in V. Then there exists a neighborhood U of v such that for all w in U, $[G_w] \preceq [G_v]$.*

Proof. Let S be a slice at v. If $w \in G \cdot S$ then w is in the orbit of a point w' in S. It follows that $G_{w'} \subset G_v$, so $[G_w] = [G_{w'}] \preceq [G_v]$. □

Definition 2.4. A vector $v \in V$ (or its orbit) is called *principal* if there exists a neighborhood U of v such that for all w in U, $[G_w] = [G_v]$. Equivalently, v is principal if it has locally minimal isotropy.

Remark 2.5.

- By definition, the set of principal points is open.

- The definition of principal points is not totally standard. Some authors, like [1, section 6] have adopted another definition: A vector $v \in V$ is principal if there exists a neighborhood U of v such that for all w in U, $[G_v] \preceq [G_w]$. Anyway, for a compact Lie group representation, the two definitions are equivalent.

Let us denote by π the canonical projection from V to V/G. The principal orbit type theorem can be stated (in the case of linear representations) as follows (see [7, Theorem 3.1], [1, section VI], [10, Theorem 2.8.5]).

Theorem 2.6 (Principal orbit type theorem)**.** *For any open subset Ω of V such that $\pi(\Omega)$ is connected, the set U_Ω of principal points in Ω is open, dense in Ω, and $\pi(U_\Omega)$ is connected.*

For the interested reader, we present a proof in Appendix B. It follows from this result that there is a unique minimal orbit type.

Definition 2.7. Let G be a compact Lie group acting linearly on V and H be an isotropy subgroup.

- The *fixed locus* V^H is defined by
$$V^H := \{v \in V;\ h \cdot v = v \text{ for all } h \in H\},$$
it is the vector subspace of elements of V fixed by H.
- The *open fixed locus* $\overset{\circ}{V}{}^H$ is the subset of V^H defined by
$$\overset{\circ}{V}{}^H := \left\{v \in V^H;\ G_v = H\right\}.$$
- The *stratum* $\Sigma_{[H]}$ is defined by
$$\Sigma_{[H]} := \{v \in V;\ [G_v] = [H]\}.$$
It is the set of vectors in V having isotropy class $[H]$ and it is the orbit of $\overset{\circ}{V}{}^H$.
- The *closed stratum*
$$\overline{\Sigma}_{[H]} = \left\{v \in V;\ gHg^{-1} \subset G_v, \text{ for some } g \in G\right\}$$
consists of vectors V having isotropy at least $[H]$. It is the orbit of V^H.

Remark 2.8.

- The terminology we use here is not totally standard, but it varies according to different authors (for instance, what we call stratum is called orbit bundle in [38]).
- The fixed locus V^H is defined for arbitrary closed subgroups of G (not only isotropy subgroups) but we will generally avoid to do so.
- The terminology "closed stratum" and the corresponding notation will be justified by corollary 2.11. The same holds for the opened fixed locus.
- The partial order relation on isotropy classes induces a (reverse) partial order relation on the strata.
$$[H_1] \preceq [H_2] \iff \Sigma_{[H_2]} \preceq \Sigma_{[H_1]}$$

The *normalizer* of H is
$$N(H) := \left\{g \in G \mid gHg^{-1} = H\right\}.$$
It is the maximal subgroup of G in which H is a normal subgroup. We have the following result (see [2], [16]):

Lemma 2.9. *For each closed subgroup H of G, V^H is $N(H)$-stable. Moreover, if $H = G_{v_0}$ is the* isotropy group *of some point $v_0 \in V$, then $N(H) = \left\{g \in G;\ g \cdot V^H \subset V^H\right\}$.*

Proof. Let v in V^H. Then, for any g in $N(H)$ and any h in H, we have
$$h \cdot (g \cdot v) = g \cdot (g^{-1}hg) \cdot v = (gh') \cdot v = g \cdot v.$$

If moreover $H = G_{v_0}$, and $g \in G$ is such that $g \cdot V^H \subset V^H$, then, $g \cdot v_0$ is in V^H and thus $H \subset gHg^{-1}$, because $G_{g\cdot v_0} = gG_{v_0}g^{-1}$. Since H is compact, $H = gHg^{-1}$ by [38, Proposition 3.7] and g belongs to $N(H)$, which ends the proof. □

The linear representation $\rho : G \to \mathrm{GL}(V)$ induces, by restriction, a linear representation of $N(H)$ on V^H

$$\rho_{N(H)} \colon N(H) \longrightarrow \mathrm{GL}(V^H).$$

This induced representation is however not faithful in general but, *when H is an isotropy group*, its kernel is exactly H and we get a *faithful* linear representation

$$\rho_{\Gamma^H} : \Gamma^H \longrightarrow \mathrm{GL}(V^H),$$

where $\Gamma^H := N(H)/H$ is called the *monodromy group* in [2]. Note that, in that case, two vectors v_1, v_2 in $V^H \cap \Sigma_{[H]}$ are in the same G-orbit if and only if they are in the same Γ^H-orbit.

Proposition 2.10. *Let H be an isotropy subgroup. Then $\overset{\circ}{V}{}^H$ is open and dense in V^H, more precisely it contains a Zariski dense open subset of V^H.*

Proof. Let x be in $\overset{\circ}{V}{}^H$. Then thanks to corollary 2.3 there exists a neighborhood U of x such that for y in U, $[G_y] \preceq [H]$. If y in $U \cap V^H$, $[H] \preceq [G_y] \preceq [H]$ so $[G_y] = [H]$. This means that $H \subset G_y = gHg^{-1}$ for some g in G so by [38, Proposition 3.7] again, $G_y = H$. This proves that $\overset{\circ}{V}{}^H$ is open. The second part is difficult and will be proven later on (see corollary 3.17). □

Corollary 2.11. *$\overline{\Sigma}_{[H]}$ is the closure of $\Sigma_{[H]}$.*

Proof. First we prove that $\overline{\Sigma}_{[H]}$ is closed. If v_n is a sequence in $\overline{\Sigma}_{[H]}$ that converges to v then there exists elements g_n in G such that $g_nHg_n^{-1} \subset G_{v_n}$. After extracting a subsequence, we can assume that g_n converges to an element g in G. Then $gHg^{-1} \subset G_v$ so v belongs to $\overline{\Sigma}_{[H]}$. Now, let v be in $\overline{\Sigma}_{[H]}$. By definition, there exists g in G such that $g^{-1} \cdot v$ belongs to V^H. Thanks to proposition 2.10, $g^{-1} \cdot v$ is the limit of a sequence of elements in $\overset{\circ}{V}{}^H$. □

For a compact Lie group representation (V, ρ), the partition into (non empty) isotropy strata

$$V = \Sigma_{[H_0]} \cup \cdots \cup \Sigma_{[H_n]}$$

is called its *isotropy stratification* or *orbit type stratification*. It can be shown that it is a real stratification, and even a Whitney stratification (see [10, §2.7 and Theorem 2.7.4]).

Example 2.12. Consider, for instance, the representation of the rotation group $G = \mathrm{SO}(3)$ on $V = S^2\mathbb{R}^3$. Then there are exactly three orbit types

$$[\mathbb{D}_2] \preceq [\mathrm{O}(2)] \preceq [\mathrm{SO}(3)],$$

where $[\mathbb{D}_2]$ is the principal orbit type. In that case, $V^{\mathbb{D}_2}$, the subspace of diagonal matrices, intersects all the orbits but since $N(\mathbb{D}_2)$ is the octahedral group $\mathbb{O}$ and the monodromy $\Gamma^{\mathbb{D}_2}$ is isomorphic to the symmetric group $\mathfrak{S}_3$, the set $V^{\mathbb{D}_2}$ is not (formally speaking) a slice, but it can be seen as a *slice with finite monodromy*.

2.2. **Invariant theory and orbits.** In the material we will present, we will constantly deal with two types of groups:

- **Compact Lie groups:** they admit automatically a faithful representation [8, Theorem III.4.1], and thanks to Weyl's unitary trick, this representation can be chosen unitary. Besides, every continuous finite-dimensional representation of G is fully irreducible, i.e. splits as a direct sum of irreducible representations.
- **Complex reductive groups:** they are complex Lie groups admitting a faithful complex analytic representations and such that every finite-dimensional analytic representation splits as a direct sum of irreducible representations.

It turns out that both type of groups are closely linked through the process of complexification, which will be detailed in 3.1. More precisely, complex reductive groups are exactly complexifications of compact Lie groups [25, Theorem 4.31]. The idea behind this link is that Weyl's unitary trick allows to prove that a complex Lie group is reductive as soon as it contains a Zariski dense compact subgroup (see for instance [24, Lemma 6.2.7]). Lastly, if $G \subset \mathrm{GL}_n(\mathbb{C})$ is reductive, then, G is automatically an algebraic subgroup of $\mathrm{GL}(n, \mathbb{C})$ [25, Theorem 5.11].

Let G be a real (resp. complex) Lie group, and let $K = \mathbb{R}$ (resp. $K = \mathbb{C}$). The linear action of G on a K-vector space V extends naturally to the polynomial algebra $K[V]$ via the formula

$$(g \cdot p)(v) := p(g^{-1} \cdot v)$$

for every polynomial $p \in K[V]$ and every vector $v \in V$. The set of all polynomials that are invariants under the action of G is a subalgebra of $K[V]$ denoted by $K[V]^G$ and called the *invariant algebra* of V.

The foundational result of invariant theory, due initially to Hilbert [20] in the case of the action of $\mathrm{GL}(n, \mathbb{C})$ on $\mathrm{Sym}^d \mathbb{C}^n$, runs as follows.

Theorem 2.13. [19, Theorem X.5.6], [24, Theorem 6.3.1] *Let G be a compact (resp. complex reductive) Lie group, let $K = \mathbb{R}$ (resp. $K = \mathbb{C}$), let V be a finite dimensional K-vector space, and let $\rho\colon G \to \mathrm{GL}(V)$ be a continuous (resp. analytic) representation of G. Then, the invariant algebra $K[V]^G$ is finitely generated. This means that there exists a finite set of invariant polynomials $p_1, \dots, p_N$ such that*

$$K[V]^G = K[p_1, \dots, p_N].$$

Remark 2.14. Although this theorem is stated most of the time for complex reductive groups (or even reductive groups over an algebraically closed field of characteristic zero), the proof in the compact case works in the same way since it relies only on the Noetherianity of $K[V]$ and the existence of a Reynolds operator (which is simply in this case obtained by averaging on the group).

It is clear that any invariant is constant on G-orbits. The geometry of orbits can be understood via the invariants, but the situation is different for the real and the complex cases.

$K = \mathbb{R}$**,** G **compact:**

- The G-orbits are compact and smooth.
- The invariants separate the G-orbits. In other terms, given two vectors $v_1, v_2 \in V$ belonging to different G-orbits, it is always possible to find a function $p \in \mathbb{R}[V]^G$ such that $p(v_1) \neq p(v_2)$ (see [1, Appendix C]).
- The orbit space V/G can be described as a semialgebraic subset of $\mathbb{R}^N$. Indeed, if $\{p_1, \dots, p_N\}$ denotes a generating set for $\mathbb{R}[V]^G$, then the mapping

$$P\colon v \mapsto \big(p_1(v), p_2(v), \dots, p_N(v)\big)$$

  induces an homeomorphism between V/G and $P(V) \subset \mathbb{R}^N$ which is a semialgebraic subset of $\mathbb{R}^N$.

$K = \mathbb{C}$**,** G **reductive:**

- The G-orbits are constructible [1], and their closure are the same for the usual or for the Zariski topology.
- Two Zariski-closed G-stable sets of V can be separated by invariants.
- Each G-orbit is adherent to a unique closed G-orbit.
- The complex scheme $V/G = \operatorname{spec} \mathbb{C}[V]^G$ parameterizes closed G-orbits.

In the same way one defines the algebra of polynomial invariants $K[V]^G$, one can define the *invariant field* $K(V)^G$ of *rational invariants*, which is a subfield of the field $K(V)$ of all rational functions on V. Note that this field is always finitely generated since it is contained in the finitely generated field $K(V)$ (see for instance [23]).

[1] A set is constructible if it is Zariski open in its Zariski closure.

Following Popov and Vinberg [34], we say that a rational invariant f separates the orbits $\mathcal{O}_1$ and $\mathcal{O}_2$ if it is defined at points of both orbits and assumes different values at these points. A subset F of $K(V)^G$ separates the orbits $\mathcal{O}_1$ and $\mathcal{O}_2$ if it contains an element that separates these orbits. Finally, we say that a subset F of $K(V)^G$ separates orbits in general position if there exists a nonempty Zariski open subset $U \subset V$ such that F separates the orbits of any two inequivalent points of U.

Theorem 2.15. [34, Lem. 2.1] *Let G be a reductive complex group and $\rho : G \to \mathrm{GL}(V)$ a complex representation of G. If a finite set $F \subset \mathbb{C}(V)^G$ separates orbits in general position, then it generates the field $\mathbb{C}(V)^G$.*

Remark 2.16.

- The converse of theorem 2.15 is also true (see [34, Theorem 2.3]) and is originally due to Rosenlicht [35].
- Theorem 2.15 is wrong in the real setting. Consider the real representation of the trivial group $G = \{e\}$ on the real space $V = \mathbb{R}$. Then the invariant field is given by $\mathbb{R}(V)^G = \mathbb{R}(x)$. The polynomial $p(x) = x^3$ separates all the orbits but is not a generator of $\mathbb{R}(V)^G$.

2.3. **The algebraic case.** The geometry of the linear action of a compact Lie group (or more generally the action of a Lie group on a manifold) has been investigated in the framework of algebraic geometry. The theory is delicate, we will present a quick overview of the situation as well as results that we need. The setting is as follows: let G be a complex reductive group acting algebraically on a complex affine algebraic variety (the theory works for any closed field of characteristic zero, but we will use it essentially in the complex case). The aim is to provide a local model for the action near an orbit of G. The most simple example happens when the action is free. If we pursue the analogy with differential geometry, we would expect a local trivialization near the orbit. However, the following example shows that it is not possible to expect such a result in the Zariski topology.

Example 2.17. Let us consider the group μ_n of n-th roots of unity, acting naturally on $\mathbb{C}^*$. In this case, the space of orbits is also isomorphic by $\mathbb{C}^*$, the quotient map π being given by $z \mapsto z^n$. We see that it is impossible to trivialize π in the Zariski topology on the base. Indeed, a Zariski open subset of $\mathbb{C}^*$ is simply obtained by removing a finite number of points, and the projection remains nontrivial on any such open subset.

The problem comes from the fact that a smooth and surjective morphism between algebraic varieties does not always have a section in the Zariski topology. However, it has a section in the etale topology [18, 17.16.3 (ii)]. Concretely this means the following: if $\varphi\colon X \to Y$ is smooth and surjective, then for any y in Y there is a neighborhood U_y of y and an etale morphism $\varphi\colon V \to U_y$ such that the pull-back morphism $\widetilde{f}\colon V \times_{U_y} X \to V$ has a section. For the interested reader, let us mention that the problem of trivializing principal G-bundles in the Zariski topology was studied in depth by Grothendieck in [17]: in fact he proved that for a given algebraic group G, then all etale locally trivial principal G-bundles are Zariski locally trivial if and only if G is affine, connected, and without torsion [17, Theorem 3].

Let us provide a very interesting example, due to Richardson, that illustrates another difficulty related to the topology of the orbits.

Example 2.18. [28, Remark 4° page 98] Let us consider the natural action of $\mathrm{SL}(2,\mathbb{C})$ on the set V_3 of cubic binary forms, *i.e.*, homogeneous complex polynomials of degree 3 in two complex variables. Now, $\mathbb{P}(V_3)$ is isomorphic to $\mathrm{S}^3\,\mathbb{P}^1$, the isomorphism being induced by the map which assigns to a cubic binary form its (unordered) three roots. The action of $\mathrm{SL}(2,\mathbb{C})$ is the natural action of $\mathrm{PGL}(2,\mathbb{C})$ on triplets of points in $\mathbb{P}^1$ after quotienting by ± 1. Hence there are only 3 possible projective orbits: $[w^3]$, $[zw^2]$ and $[z(w-z)w]$, whose respective stabilizers in $\mathrm{PGL}(2,\mathbb{C})$

are

$$\mathrm{PGL}(2,\mathbb{C})_{[w^3]} = \left\{ \begin{pmatrix} a & b \\ 0 & 1 \end{pmatrix}, a \in \mathbb{C}^*, b \in \mathbb{C} \right\},$$
$$\mathrm{PGL}(2,\mathbb{C})_{[zw^2]} = \left\{ \begin{pmatrix} a & 0 \\ 0 & 1 \end{pmatrix}, a \in \mathbb{C}^* \right\}$$
$$\mathrm{PGL}(2,\mathbb{C})_{[z(1-z)w]} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix}, \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix} \right\}.$$

We can now look at the pre-images of these stabilizers in $\mathrm{SL}(2,\mathbb{C})$. They act by characters on binary forms. More precisely, for ε in $\{-1,+1\}$, if we denote by $\gamma \star f$, the right action of $\gamma \in \mathrm{SL}(2,\mathbb{C})$ on $f \in V_3$, given by $(\gamma \star f)(\xi) = f(\gamma \cdot \xi)$, where $\xi = (z,w)$, we get

$$\begin{pmatrix} \alpha & \beta \\ 0 & 1/\alpha \end{pmatrix} \star w^3 = \frac{w^3}{\alpha^3}, \qquad \begin{pmatrix} \alpha & 0 \\ 0 & 1/\alpha \end{pmatrix} \star zw^2 = \frac{zw^2}{\alpha}$$
$$i\varepsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \star z(w-z)w = -i\varepsilon z(w-z), \qquad i\varepsilon \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} \star z(w-z)w = -i\varepsilon z(w-z)$$
$$\varepsilon \begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix} \star z(w-z)w = -\varepsilon z(w-z)w, \qquad i\varepsilon \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix} \star z(w-z)w = i\varepsilon z(w-z)w$$
$$\varepsilon \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix} \star z(w-z)w = -\varepsilon z(w-z)w.$$

Hence we have 4 orbit types:

- The orbit of 0 has stabilizer $\mathrm{SL}(2,\mathbb{C})$.
- The orbit of w^3 has stabilizer $\mathbb{C} \rtimes \mathbb{Z}/3\mathbb{Z}$.
- The orbit of zw^2 has trivial isotropy.
- The orbit of $z(w-z)w$ has isotropy

$$\left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix} \right\} \simeq \mathbb{Z}/3\mathbb{Z}.$$

Now, the set U of binary forms which have three distinct roots is a Zariski open subset of V_3 defined by the non vanishing of the discriminant. It is dense, and all points in U have isotropy $\mathbb{Z}/3\mathbb{Z}$. However, $\mathrm{SL}(2;\mathbb{C})_{zw^2}$ is trivial. Hence the generic orbit has isotropy $\mathbb{Z}/3\mathbb{Z}$, but another orbit type has trivial stabilizer. This example shows that we cannot expect corollary 2.3 to be true in whole generality in the algebraic setting.

In the preceding example, the reason why this problem occurs is that the orbit of zw^2 is not closed. In the case of a closed orbit, Luna's slice theorem gives a good description of the situation.

Theorem 2.19. [28] *Let G be a reductive group acting on an affine algebraic variety X. Let x be a point of X and assume that the orbit $G \cdot x$ is closed in X. Then there exists an etale slice at x, that is an affine subvariety V of X passing through x satisfying the following properties:*

- *V is G_x-stable*
- *The natural G-morphism $\varphi\colon G \times_{G_x} V \to U$ is etale, and its image U is an affine neighborhood of the orbit $G \cdot x$.*

Using this theorem, Luna was able to recover results that were holding in the case of compact Lie group actions, like finiteness of orbit types. The result that will be of crucial importance for us is the algebraic version of corollary 2.3.

Corollary 2.20. [28, Remark 4° pp. 98] *Let G be a reductive group acting on an affine algebraic variety X. Let x be a point of X and assume that the orbit $G \cdot x$ is closed in X. Then there exists a Zariski open neighborhood of x such that for any y in X, G_y is conjugate to a subgroup of G_x.*

3. Complexification

3.1. **Complexification of a compact Lie group.** The complexification of a real Lie group is formally defined as the solution of a universal problem, which always exists and is unique up to a complex analytic isomorphism ([6, Chapter 3]).

If G is compact, it is possible to define $G^{\mathbb{C}}$ as follows (see [8, III.8]): let $\mathcal{A}$ be the algebra of representative functions on G, that is functions that generate a finite-dimensional representation inside $\mathcal{C}^0(A,\mathbb{R})$. Tannaka-Krein duality [8, III.7] guarantees that G identifies with real characters of $\mathcal{A}$, that is every character of $\mathcal{A}$ is of the form $f \to f(g)$ for g in G. Then $G^{\mathbb{C}}$ is defined as the complex characters of $\mathcal{A}^{\mathbb{C}}$.

Example 3.1. If $G = \mathrm{U}(1)$, $\mathcal{A}$ is the algebra of trigonometric polynomials $\mathbb{R}[\cos(\theta),\sin(\theta)]$. Its complexification is the algebra $\mathbb{C}[\cos(\theta),\sin(\theta)]$. Given a complex polynomial $P(\cos\theta,\sin\theta)$, we can associate the Laurent Polynomial $P\left(\frac{z+1/z}{2},\frac{z-1/z}{2i}\right)$. In this way we see that

$$\mathbb{C}[\cos(\theta),\sin(\theta)] \simeq \mathbb{C}[z,1/z],$$

since every Laurent polynomial is uniquely determined by its restriction on $\mathrm{U}(1)$. Hence, the complex characters of $\mathbb{C}[\cos(\theta),\sin(\theta)]$ are exactly the points of $\mathbb{C}^*$.

There is an explicit way to describe this complexification, which is pretty useful to understand more precisely the geometry of $G^{\mathbb{C}}$. To achieve this, we use the fact that every compact Lie group admits a faithful representation [8, Thm. III.4.1], and thanks to Weyl's unitary trick, it admits a faithful unitary representation. Before going further, let us recall some elementary facts of linear algebra.

Lemma 3.2.

(1) *Polar decomposition: if* $\mathrm{P}(n)$ *denotes the set of hermitian positive definite matrices, then the product map*
$$\mathrm{U}(n)\times\mathrm{P}(n) \xrightarrow{\sim} \mathrm{GL}(n,\mathbb{C})$$
is a diffeomorphism.

(2) *If* ι *denotes the Cartan involution* $M \to (M^*)^{-1}$ *of* $\mathrm{GL}(n,\mathbb{C})$*, then for any* M *in* $\mathrm{GL}(m,\mathbb{C})$ *with polar decomposition* gh*,* $h^2 = \iota(M)^{-1}M$*.*

(3) $\mathrm{U}(n) = \{M \in \mathrm{GL}(n,\mathbb{C}), \iota(M) = M\}$ *and* $\mathrm{P}(n) = \{M \in \mathrm{GL}(n,\mathbb{C}), \iota(M) = M^{-1}\}$*.*

(4) *The map* $Z \to e^{iZ}$ *from* $\mathfrak{u}(n)$ *to* $\mathrm{P}(n)$ *is a diffeomorphism, where* $\mathfrak{u}(n) = \mathrm{Lie}(\mathrm{U}(n))$ *is the Lie algebra of skew-hermitian matrices.*

This being done, the complexification of a compact Lie group can be described as follows.

Proposition 3.3. [8, Prop. III.8.3] *Let* $G \subset \mathrm{U}(n)$ *be a compact Lie group and let* $\mathfrak{g}$ *be its Lie algebra. Then*
$$G^{\mathbb{C}} = \left\{ge^{iZ}\ ;\ g \in G \text{ and } Z \in \mathfrak{g}\right\}$$
In particular, $G^{\mathbb{C}}$ *is diffeomorphic to* $G \times \mathfrak{g}$*.*

Remark 3.4. This result might be surprising at first glance because it is not clear at all that the right hand side is a group. Let us briefly explain by hand why it is the case. Given $g_1e^{iZ_1}$ and $g_2e^{iZ_2}$, where $g_1, g_2 \in G$ and $Z_1, Z_2 \in \mathfrak{g}$, we have

$$e^{iZ_1}g_2 = g_2\mathrm{Ad}(g_2^{-1})e^{iZ_1} = g_2e^{i\mathrm{Ad}(g_2^{-1})(Z_1)} = g_2e^{iZ_3},$$

where $Z_3 \in \mathfrak{g}$. We get thus $g_1e^{iZ_1}g_2e^{iZ_2} = g_1g_2e^{iZ_2}e^{iZ_3}$. Writing
$$e^{iZ_2}e^{iZ_3} = ge^{iZ},$$
with $g \in \mathrm{U}(n)$ and $Z \in \mathfrak{u}(n)$, we have thanks to lemma 3.2 (2),
$$e^{2iZ} = \iota(e^{iZ_2}e^{iZ_3})^{-1}e^{iZ_2}e^{iZ_3} = e^{iZ_3}e^{2iZ_2}e^{iZ_3}.$$

Consider now the real analytic function

$$\varphi\colon \mathfrak{g}\times\mathfrak{g} \to \mathfrak{u}(n), \qquad (Z_2,Z_3) \mapsto \frac{1}{2i}\log(e^{iZ_3}e^{2iZ_2}e^{iZ_3}).$$

By applying lemma A.1 two times, we get that $\varphi(Z_2, Z_3) \in \mathfrak{g}^{\mathbb{C}}$ for sufficiently small Z_2, Z_3 and by corollary A.5, we conclude that for all Z_2, Z_3 in $\mathfrak{g}$, $\varphi(Z_2, Z_3) \in \mathfrak{g}^{\mathbb{C}} \cap \mathfrak{u}(n) = \mathfrak{g}$. Hence this proves that for all Z_2, Z_3 in $\mathfrak{g}$, Z is in $\mathfrak{g}$.

We can apply again the same trick: consider the real analytic map

$$\Psi\colon \mathfrak{g} \times \mathfrak{g} \to \mathrm{U}(n), \qquad (Z_2, Z_3) \mapsto e^{iZ_2} e^{iZ_3} e^{-i\varphi(Z_2,Z_3)}.$$

For Z_2, Z_3 close to 0, $\log \Psi$ takes values in $\mathfrak{g}^{\mathbb{C}} \cap \mathfrak{u}(n) = \mathfrak{g}$, so Ψ takes values in G. As G is a closed real analytic submanifold of $\mathrm{U}(n)$ by corollary A.2, we deduce using again corollary A.5 that for all Z_2, Z_3 in $\mathfrak{g}$, $\Psi(Z_2, Z_3) \in G$. Since $\Psi(Z_2, Z_3) = g$, we deduce that g belongs to G and we are done.

Remark 3.5. The group G is a closed subgroup of $\mathrm{GL}(n; \mathbb{C})$, and it is straightforward to check that $\mathrm{Lie}(G^{\mathbb{C}}) = \mathfrak{g} + i\mathfrak{g} = \mathfrak{g}^{\mathbb{C}}$ since $\mathfrak{u}(n)$ is totally real in $\mathfrak{gl}(n; \mathbb{C})$. Hence $\mathrm{Lie}(G^{\mathbb{C}})$ carries a natural complex structure for which the bracket is complex linear. It defines on $G^{\mathbb{C}}$ a complex Lie group structure for which the exponential map is a local biholomorphism around 0. Besides, G is totally real in $G^{\mathbb{C}}$.

We have an even stronger property :

Proposition 3.6. *The complexified group $G^{\mathbb{C}}$ is an affine algebraic subvariety of* $\mathrm{GL}(n, \mathbb{C})$.

Proof. This is [8, Prop. III.8.2], the key point being the fact that the algebra of representative functions on G is finitely generated. □

Corollary 3.7. *If G is a compact Lie group, then G is analytically Zariski dense in $G^{\mathbb{C}}$.*

Proof. The group G is a totally real analytic submanifold of $G^{\mathbb{C}}$. Hence, thanks to corollary A.2, the Zariski closure of G in $G^{\mathbb{C}}$ is the union of connected components of $G^{\mathbb{C}}$ that contain G. By Proposition 3.3, this union is $G^{\mathbb{C}}$ itself. □

Corollary 3.8. *Let G be a compact Lie group, and assume that $G^{\mathbb{C}}$ acts holomorphically on a (non-necessarily finite dimensional) complex vector space W. Then $W^{G^{\mathbb{C}}} = W^G$.*

Proof. For w in W^G, let us consider a linear form u on W. Let $\phi\colon G^{\mathbb{C}} \to \mathbb{C}$ given by $\phi(g) = u(g \cdot w - w)$. Then ϕ is holomorphic and ϕ vanishes on G. Thanks to corollary 3.7, ϕ vanishes on $G^{\mathbb{C}}$. This means that for all g in $G^{\mathbb{C}}$, all linear forms take the same values on w and $g \cdot w$, so $g \cdot w = w$. Hence w is fixed by $G^{\mathbb{C}}$. □

Finally, let us prove that $G^{\mathbb{C}}$ satisfies a universal property (which is more general than [8, Proposition III.8.6] which concerns only linear representations).

Proposition 3.9. *Let G be a compact Lie group, $G^{\mathbb{C}}$ its complexification, and $\phi\colon G \to G^{\mathbb{C}}$ the natural morphism. For any complex Lie group H and any morphism $f\colon G \to H$ of Lie groups, there exists a unique homomorphism $F : G^{\mathbb{C}} \to H$ of complex Lie groups such that $f = F \circ \phi$.*

$$\begin{tikzcd} G \arrow[r, "f"] \arrow[d, "\phi"'] & H \\ G^{\mathbb{C}} \arrow[ur, "F"'] & \end{tikzcd}$$

Proof. We use the notation of proposition 3.3. Let σ denote the differential of f at the origin and let $\sigma^{\mathbb{C}}\colon \mathfrak{g}^{\mathbb{C}} \to \mathfrak{h}$ be its complexification. We define a map $F\colon G^{\mathbb{C}} \to H$ by $F(ge^{iZ}) = f(g)e^{i\sigma(Z)}$.

First we claim that F is holomorphic. By Lie's third theorem (see [37, §II.8, Thm 1]), the morphism $\sigma^{\mathbb{C}}$ can be uniquely integrated to a local holomorphic group morphism $\widetilde{F}\colon G^{\mathbb{C}} \dashrightarrow H$ defined in a neighborhood of the identity, whose differential at the identity element is $\sigma^{\mathbb{C}}$. Hence, $\widetilde{F}_{|G}$ integrates σ, so $\widetilde{F}_{|G} = f$. Hence, for g close to the identity and Z close to 0, we get

$$\widetilde{F}(ge^{iZ}) = \widetilde{F}(g)\widetilde{F}(e^{iZ}) = f(g)e^{\sigma^{\mathbb{C}}(iZ)} = f(g)e^{i\sigma(Z)} = F(ge^{iZ}),$$

so $F = \widetilde{F}$ near the identity. It follows that F is holomorphic near the identity. Since F is real analytic, F is holomorphic on $(G^{\mathbb{C}})^e$. Since for g in G and ℓ in $G^{\mathbb{C}}$, $F(g\ell) = f(g)F(\ell)$, it follows that F is holomorphic on $G^{\mathbb{C}}$. Lastly, $F_{|G} = f$ is a group morphism on G, so by corollary 3.7, applied two times, F is a group morphism. □

3.2. **Complexification of a real representation.** Let $\rho : G \to \mathrm{GL}(V)$ be a real continuous representation of a compact Lie group G. By proposition 3.9, there exists a unique analytic extension

$$\rho^{\mathbb{C}} : G^{\mathbb{C}} \to \mathrm{GL}(V^{\mathbb{C}})$$

of ρ. This complexified representation enjoys some very specific properties that we will list below.

Proposition 3.10. *If we see $G^{\mathbb{C}}$ as an affine algebraic group (via proposition 3.6), then $\rho^{\mathbb{C}}$ is an algebraic map.*

Proof. This is proved in [8, Proposition III.8.6]. □

Remark 3.11. The link between compacity and algebraicity is a beautiful result that relies on the Peter-Weyl theorem and on the finiteness of the algebra of representative functions. Outside of this context, such results become immediately wrong. For instance, $\mathbb{C}$ and $\mathbb{C}^\times$ are both complex affine algebraic groups, but $\exp\colon \mathbb{C} \to \mathbb{C}^\times$ is a holomorphic Lie group morphism that is no longer algebraic. This comes from the fact that $\mathbb{C}$ is not reductive.

Proposition 3.12. *Given (V, G), there exists a $G^{\mathbb{C}}$-stable and nonempty Zariski open subset U of $V^{\mathbb{C}}$ such that all orbits of points in U are closed.*

Proof. Since G is compact, we can endow V with an inner product. Hence we have a chain of maps

$$G \xrightarrow{\rho} O(n) \subset \mathrm{U}(n) \subset GL(n; \mathbb{C})$$

Thanks to proposition 3.3, it is possible to check that $O(n)^{\mathbb{C}} = O(n; \mathbb{C})$ so we get that $\rho^{\mathbb{C}}$ takes values in $O(n; \mathbb{C})$. Hence the action preserves a symmetric nondegenerate complex bilinear form, and the result follows from [27]. □

Lemma 3.13. *For any v in V, $(G^{\mathbb{C}})_v = (G_v)^{\mathbb{C}}$.*

Proof. By corollary 3.7, G_v is Zariski dense in $(G_v)^{\mathbb{C}}$ so $(G_v)^{\mathbb{C}}$ fixes v for the complexified representation. This yields the inclusion $(G_v)^{\mathbb{C}} \subset (G^{\mathbb{C}})_v$.

For the converse implication, we argue as in the proof of proposition 3.12. Let us denote by $d\rho$ the differential of the G-action at the origin. Let $\ell = ge^{iZ}$ be an element of $(G^{\mathbb{C}})_v$. Then $\iota(\ell)$ belongs to $(G^{\mathbb{C}})_v$ too, so $e^{2iZ} = \iota(\ell)^{-1}\ell$ belongs to $(G^{\mathbb{C}})_v$. It means that $\exp(2i\, d\rho(Z)) \cdot v = v$. Now $2i\, d\rho(Z)$ is a complex hermitian endomorphism of V, so it is diagonalizable with real eigenvalues. It follows that $d\rho(Z)(\ell) = 0$, so Z belongs to $\mathrm{Lie}(G_v)$. Hence, e^{iZ} fixes v so g fixes v too. It follows that g belongs to G_v, which proves that ℓ belongs to $(G_v)^{\mathbb{C}}$. □

Proposition 3.14. *For any v in V, $G^{\mathbb{C}} \cdot v$ is closed.*

Proof. It follows directly from [11, Lemma 2.2] since G is compact. □

Remark 3.15. For the reader's convenience, we can provide a sketch of the proof of the above proposition. It relies heavily on the beautiful theory of Kempf and Ness [22]. Let us fix an inner product on V such that G acts by orthogonal transformations, and extend it to an hermitian product on $V^{\mathbb{C}}$. The moment map $\mu\colon V^{\mathbb{C}} \to \mathfrak{g}^*$ is given by

$$\mu(v)(\xi) = \frac{1}{2i}\langle \xi \cdot v | v \rangle$$

This definition makes sense because ξ belongs to $\mathfrak{u}(V^{\mathbb{C}})$ so it is skew-hermitian. Then Kempf-Ness theorem states that an orbit $G^{\mathbb{C}} \cdot v$ is closed if and only $G^{\mathbb{C}} \cdot v \cap \mu^{-1}(0) \neq \emptyset$ (see for instance [26, Theorem 4]). However, since G acts by orthogonal transformations, the moment map μ vanishes on V. The result follows.

Proposition 3.16. *For any isotropy H, the complex open fixed locus in $(V^{\mathbb{C}})^{H^{\mathbb{C}}}$ contains a nonempty Zariski open set.*

Proof. Let v be a vector in V such that $G_v = H$. Thanks to proposition 3.14, $G^{\mathbb{C}} \cdot v$ is closed, and thanks to corollary 2.20, there exists a Zariski open set U containing x such that for any w in U, G_w is conjugate to a subgroup of G_v. Let us now look at $\widetilde{U} = U \cap (V^{\mathbb{C}})^{H^{\mathbb{C}}}$, which is a nonempty Zariski open subset of $(V^{\mathbb{C}})^{H^{\mathbb{C}}}$. Then for w in $\widetilde{U}$, $(G^{\mathbb{C}})_w$ is conjugate to a subgroup of $H^{\mathbb{C}}$ so there exists g in $G^{\mathbb{C}}$ such that

$$H^{\mathbb{C}} \subset (G^{\mathbb{C}})_w \subset g^{-1} H^{\mathbb{C}} g.$$

It follows from lemma A.3 that g normalizes $H^{\mathbb{C}}$, which implies that $(G^{\mathbb{C}})_w = H^{\mathbb{C}}$. □

Corollary 3.17. *For any isotropy H, the open fixed locus $\overset{\circ}{V}{}^H$ contains a nonempty (real) Zariski open set.*

Proof. Thanks to corollary 3.8 we have $(V^H)^{\mathbb{C}} = (V^{\mathbb{C}})^H = (V^{\mathbb{C}})^{H^{\mathbb{C}}}$. Then the result follows from proposition 3.16 and corollary A.7. □

We can also compare real and complex orbits. This result won't be strictly necessary in the sequel but it can help to understand the geometry of the situation.

Proposition 3.18. *For any vector v in V, $(G^{\mathbb{C}} \cdot v) \cap V = G \cdot v$.*

Proof. One inclusion is obvious. For the other inclusion, let H be the isotropy of v. Thanks to lemma 3.13, the orbit $G^{\mathbb{C}} \cdot v$ is isomorphic to $G^{\mathbb{C}}/H^{\mathbb{C}}$. Let ι denotes the Cartan involution on $G^{\mathbb{C}}$. Assume that $\ell \cdot v$ is real for some element ℓ in $G^{\mathbb{C}}$. Then $\iota(\ell) \cdot v = \overline{\ell \cdot v} = v$ so $\iota(\ell)^{-1}\ell$ belongs to $H^{\mathbb{C}}$. If $\ell = ge^{iZ}$, then e^{2iZ} belongs to $H^{\mathbb{C}}$. It implies that Z is in $\mathfrak{h}$, so e^{iZ} is in $H^{\mathbb{C}}$. Hence $\ell \cdot v = g \cdot v$. □

Remark 3.19. The result [5, Proposition 2.3] predicts in our case that the intersection of a complex orbit with real points is a *finite union* of real orbits. Hence this result is weaker, but holds for more general groups.

Example 3.20. Let us give an example where this intersection is strictly bigger than the real orbit. For this we take again Example 2.18, but with the action of $\mathrm{GL}(2;\mathbb{C})$ instead of $\mathrm{SL}(2;\mathbb{C})$ acting on the vector space of degree 3 binary forms. Then the $\mathrm{GL}(2,\mathbb{R})$-orbit of $z(w-z)w$ consists of all binary forms of degree 3 with real coefficients and 3 distinct roots. However, real binary forms that are in the $\mathrm{GL}(2,\mathbb{C})$-orbit of $z(w-z)w$ consist of real binary forms with 3 distinct roots (not necessarily real). This locus is a union of two $\mathrm{GL}(2;\mathbb{R})$ orbits: the orbit of $z(w-z)w$ and the orbit of $z(z^2+w^2)$. There is no contradiction with the result we proved, because $\mathrm{GL}(2,\mathbb{R})$ is not compact. As a matter of fact, $\mathrm{GL}(2,\mathbb{R})$ is the split real form of $\mathrm{GL}(2,\mathbb{C})$ and not the compact one, which is $\mathrm{U}(2)$.

Finally, we go back to the algebra of invariants.

Lemma 3.21. *The three complex algebras $(\mathbb{R}[V]^G)^{\mathbb{C}}$, $\mathbb{C}[V^{\mathbb{C}}]^G$ and $\mathbb{C}[V^{\mathbb{C}}]^{G^{\mathbb{C}}}$ are naturally isomorphic.*

Proof. We have $\mathbb{R}[V]^{\mathbb{C}} \simeq \mathbb{C}[V^{\mathbb{C}}]$. Then the result follows from corollary 3.8. □

Corollary 3.22. *If $\{J_1, \ldots, J_N\}$ is a set of generators for $\mathbb{R}[V]^G$, then, it is also a generating set for $\mathbb{C}[V^{\mathbb{C}}]^{G^{\mathbb{C}}}$.*

3.3. **Complexification of normalizers.** The aim of this section is to prove that the complexification of the normalizer of a compact subgroup of a compact Lie group is naturally isomorphic to the normalizer of the corresponding complexified subgroup (proposition 3.26). This result is in accordance with Luna's result [30, Lemma 1.1]. In the following three lemmas, G denotes a compact Lie group acting on a vector space V and H is a Lie subgroup of G. We denote by $G^{\mathbb{C}}$ and $H^{\mathbb{C}}$ their respective complexifications.

Lemma 3.23. *Let H be a closed subgroup of a Lie group G and let Γ be a set of representatives in H of the finite group H/H^e, where H^e is the identity component of H. Then,*

$$\mathrm{Lie}(N(H)) = N(\mathfrak{h}) \cap \{X \in \mathfrak{g},\ \forall \gamma \in \Gamma,\ \mathrm{Ad}(\gamma)(X) - X \in \mathfrak{h}\}.$$

Proof. Let $X \in \mathrm{Lie}(N(H))$ then for all real t, e^{tX} is in $N(H)$. Let $Y \in \mathfrak{h}$, then e^{sY} is in H and therefore $\mathrm{Ad}(e^{tX})(e^{sY})$ is in H. Taking the derivatives with respect to s and then to t, we get $\mathrm{Ad}(X)(Y) \in \mathfrak{h}$ which implies that $X \in N(\mathfrak{h})$. Now, let γ be in Γ. Then $\mathrm{Ad}(e^{tX})(\gamma)$ belongs to the connected component $H^e\gamma$ of H containing γ. Consequently, $e^{tX}\gamma e^{-tX}\gamma^{-1} \in H$. Deriving at $t = 0$ we get that $X - \mathrm{Ad}(\gamma)(X)$ is in $\mathfrak{h}$.

Conversely, let $X \in N(\mathfrak{h}) \cap \{X \in \mathfrak{g},\ \forall \gamma \in \Gamma,\ \mathrm{Ad}(\gamma)(X) - X \in \mathfrak{h}\}$, and let Y be in $\mathfrak{h}$. Then,

$$e^{tX}e^{sY}e^{-tX} = \mathrm{Ad}(e^{tX})(e^{sY}) = e^{s\,\mathrm{Ad}(e^{tX})(Y)} = e^{s\exp(t\mathrm{ad}(X))(Y)} \in H.$$

It follows that $e^{tX}H^e e^{-tX} \subset H^e$. We must now deal with the other connected components. Let γ be in Γ. Then

$$e^{tX}\gamma e^{-tX}\gamma^{-1} = e^{tX}\,\mathrm{Ad}(\gamma)(e^{-tX}) = e^{tX}e^{-\mathrm{Ad}(\gamma)(tX)} = e^{tX}e^{t(X-\mathrm{Ad}(\gamma)(X))-tX}.$$

Set $Y = X - \mathrm{Ad}(\gamma)(X)$, then, by assumption, $Y \in \mathfrak{h}$ and $tY - tX = -\mathrm{Ad}(\gamma)(X) \in \mathfrak{h}$. By applying Baker-Campbell-Hausdorff formula (lemma A.1) on $e^{tX}\gamma e^{-tX}\gamma^{-1} = e^{tX}e^{tY-tX}$, we get that $e^{tX}\gamma e^{-tX}\gamma^{-1} = e^{tZ}$ where Z is an iteration of Lie brackets in terms of X and Y hence $Z \in \mathfrak{h}$. Therefore, we have

$$e^{tX}(\gamma e^{sY})e^{-tX} = \underbrace{(e^{tX}\gamma e^{-tX})\gamma^{-1}}_{\in H}\gamma\underbrace{(e^{tX}e^{sY}e^{-tX})}_{\in H^e} \in H.$$

Consequently, e^{tX} normalizes H, which implies that X belongs to $\mathrm{Lie}(N(H))$. □

Lemma 3.24. *Let $\mathfrak{h}$ be a Lie subalgebra of $\mathfrak{u}(n)$, $Z \in \mathfrak{h}$, $B \in N(\mathfrak{h})$ and $A \in \mathfrak{u}(n)$.*

$$\textit{If } e^{2iA} = e^{iB}e^{iZ}e^{iB} \quad \textit{then} \quad A - B \in \mathfrak{h}.$$

Proof. Consider the following real analytic function

$$f\colon \mathfrak{u}(n) \times N(\mathfrak{h}) \to \mathfrak{u}(n), \qquad (Z, B) \mapsto \frac{1}{i}\ln(e^{iB}e^{iZ}e^{iB}) - 2B.$$

Note that f is well-defined because $e^{iB}e^{iZ}e^{iB}$ is an element of $\mathrm{P}(n)$, thanks to lemma 3.2 (2). Indeed,

$$\iota(e^{iB}e^{iZ}e^{iB}) = e^{-iB}e^{-iZ}e^{-iB} = (e^{iB}e^{iZ}e^{iB})^{-1}.$$

Then, we can take its logarithm in $\mathfrak{u}(n)$ thanks to lemma 3.2 (3). Next, we apply Baker-Campbell-Hausdorff formula (lemma A.1) two times on $e^{iB}e^{iZ}e^{iB}$ and we deduce that $f(B, Z)$ is in $\mathfrak{h}$ for B and Z sufficiently close to zero. Thanks to corollary A.5, this is valid everywhere since f is real analytic. Hence $A - B$ belongs to $\mathfrak{h}$. □

Finally, we need the following classical result.

Lemma 3.25. *Let u be a diagonalizable endomorphism of a vector space V with real eigenvalues. If $W \subset V$ is stable by $\exp(u)$, then W is stable by u.*

Proof. Let $\lambda_1, \dots, \lambda_k$ be the distinct eigenvalues of u, and let P be a polynomial such that for any i, $P(e^{\lambda_i}) = \lambda_i$. Then $P(\exp(u)) = u$, since this equality can be checked on a basis of eigenvectors of u. The result follows directly. □

Proposition 3.26. *We have*

$$N_{G^{\mathbb{C}}}(H^{\mathbb{C}}) = (N_G(H))^{\mathbb{C}}.$$

Proof. If g is in $N_G(H)$, then, $gHg^{-1} \subset H \subset H^{\mathbb{C}}$. Consider the holomorphic application

$$C_g\colon H^{\mathbb{C}} \to G^{\mathbb{C}}/H^{\mathbb{C}}, \qquad h \mapsto ghg^{-1}.$$

Then, C_g vanishes on H, and thanks to corollary 3.7, C_g vanishes on $H^{\mathbb{C}}$. The same argument applies for g^{-1} so g normalizes $H^{\mathbb{C}}$ in $G^{\mathbb{C}}$. Hence $N_G(H) \subset N_{G^{\mathbb{C}}}(H^{\mathbb{C}})$ and by theorem 3.3 we get

$$(N_G(H))^{\mathbb{C}} \subset N_{G^{\mathbb{C}}}(H^{\mathbb{C}}).$$

Let us prove the reverse inclusion. Let g be in $N_{G^{\mathbb{C}}}(H^{\mathbb{C}})$. By theorem 3.3, we can write $g = ke^{iX}$ with k in G and X in $\mathfrak{g}$. We need to prove that k (resp. X) belongs to $N(H)$ (resp. $\mathrm{Lie}(N(H))$. We have $\iota(g) = ke^{-iX}$. To prove that $X \in \mathrm{Lie}(N(H))$, we use the description of $\mathrm{Lie}(N(H))$ given in lemma 3.23.

On one hand, thanks to lemma 3.2 (2), we have $e^{2iX} = \iota(g)^{-1}g$. Besides, the normalizer of $H^{\mathbb{C}}$ is stable under the Cartan involution ι, and hence e^{2iX} normalizes $H^{\mathbb{C}}$. This implies that $\mathrm{Ad}(e^{2iX})(\mathfrak{h}^{\mathbb{C}}) = \mathfrak{h}^{\mathbb{C}}$, where $\mathfrak{h}$ is the Lie algebra of H. Now $\mathrm{Ad}(e^{2iX}) = \exp(2i\mathrm{ad}(X))$. Since X is in $\mathrm{u}(n)$, $2i\mathrm{ad}(X)$ is diagonalizable with real eigenvalues. Thanks to lemma 3.25, $\mathrm{ad}(X)(\mathfrak{h}^{\mathbb{C}}) \subset \mathfrak{h}^{\mathbb{C}}$. Consequently, $X \in N(\mathfrak{h}^{\mathbb{C}})$. Since X is in $\mathfrak{u}(n)$, X belongs to $N(\mathfrak{h})$.

On the other hand, let γ in Γ. Then $e^{2iX}\gamma e^{-2iX} \in H^{\mathbb{C}}$ since $e^{2iX} \in N(H^{\mathbb{C}})$. Now we calculate $\iota(e^{2iX}\gamma e^{-2iX})^{-1}(e^{2iX}\gamma e^{-2iX})$ which on one side gives e^{2iZ} with $Z \in \mathfrak{h}$ and on the other side, we have

$$\begin{aligned}\iota(e^{2iX}\gamma e^{-2iX})^{-1}(e^{2iX}\gamma e^{-2iX}) &= (e^{-2iX}\gamma e^{2iX})^{-1}(e^{2iX}\gamma e^{-2iX})\\ &= e^{-2iX}\,\mathrm{Ad}(\gamma^{-1})(e^{4iX})e^{-2iX}\\ &= e^{-2iX}e^{4i\,\mathrm{Ad}(\gamma^{-1})(X)}e^{-2iX}.\end{aligned}$$

Therefore, combining the two equalities together, we get

$$e^{2iZ} = e^{-2iX}e^{4i\,\mathrm{Ad}(\gamma^{-1})(X)}e^{-2iX}$$

that is

$$e^{4i\,\mathrm{Ad}(\gamma^{-1})(X)} = e^{2iX}e^{2iZ}e^{2iX}.$$

Applying lemma 3.24 with $A = 2\,\mathrm{Ad}(\gamma^{-1})(X) \in \mathfrak{u}(n)$ and $B = 2X \in N(\mathfrak{h})$, we have finally $\mathrm{Ad}(\gamma^{-1})(X) - X \in \mathfrak{h}$, so $X - \mathrm{Ad}(\gamma)(X) \in \mathfrak{h}$. This proves that X belongs to $\mathrm{Lie}(N(H))$.

Now, both e^{iX} and ke^{iX} normalize $H^{\mathbb{C}}$ and so does $k \in N(H^{\mathbb{C}})$. We have $kH^{\mathbb{C}}k^{-1} = H^{\mathbb{C}}$ so

$$H = H^{\mathbb{C}} \cap \mathrm{U}(n) = kH^{\mathbb{C}}k^{-1} \cap \mathrm{U}(n) = k(H^{\mathbb{C}} \cap \mathrm{U}(n))k^{-1} = kHk^{-1}$$

so k belongs to $N_G(H)$. □

4. Proof of the main theorem

The main idea to prove theorem 1.1 is issued from the following erroneous proof. Let $\{J_1, \dots, J_N\}$ be a generating set for the invariant algebra $\mathbb{R}[V]^G$. Then this set is a separating set for (V, G) (see the discussion after remark 2.14). For $1 \le k \le N$, let j_k denote the restriction of J_k to V^H. The inclusion $V^H \hookrightarrow V$ induces the morphism

$$\mathbb{R}[V]^G \to \mathbb{R}[V^H]^{N(H)}, \qquad \{J_1, \dots, J_N\} \mapsto \{j_1, \dots, j_N\}.$$

Then, the set $\{j_1, \dots, j_N\}$ is separating for $(V^H, N(H))$. If theorem 2.15 was true for a real representation, we could conclude that F is a generating set for the invariant field $\mathbb{R}(V^H)^{N(H)}$ and this would achieve the proof. Unfortunately this is false. However, this argument can be modified to become a real proof.

Proof of theorem 1.1. Let $\{J_1, \dots, J_N\}$ be a generating set for the invariant algebra $\mathbb{R}[V]^G$. Then $\{J_1, \dots, J_N\}$ separates the orbits of (V, G). Let j_k be the restriction of J_k on V^H, then, the j_k separate the orbits of $V^H \cap \Sigma_{[H]}$.

Let $W = (V^{\mathbb{C}})^{H^{\mathbb{C}}}$. Thanks to proposition 3.16, there exists a nonempty Zariski open set U_1 of W such that for any w in U_1, $G_w^{\mathbb{C}} = H^{\mathbb{C}}$. Let $K = N_G(H)$. The group K acts on W, and thanks to proposition 3.12, there exists a nonempty Zariski open subset U_2 of W such that all $K^{\mathbb{C}}$-orbits of elements of U_2 are closed in W. Let $U = U_1 \cap U_2$, then, U is also a nonempty Zariski open set in W.

We claim that $\{j_1, \dots, j_N\}$ separates $K^{\mathbb{C}}$-orbits of elements in U. To prove this, let w_1 and w_2 be two elements in U that are not in the same $K^{\mathbb{C}}$-orbit. Assume that w_2 and w_1 are in the same $G^{\mathbb{C}}$-orbit. If $gw_1 = w_2$ for some g in $G^{\mathbb{C}}$, then $H^{\mathbb{C}} = gH^{\mathbb{C}}g^{-1}$ and g belongs to $N_{G^{\mathbb{C}}}(H^{\mathbb{C}})$. Thanks to proposition 3.26, g is in $K^{\mathbb{C}}$, which gives a contradiction. Hence $G^{\mathbb{C}}w_1 \cap G^{\mathbb{C}}w_2 = \emptyset$.

The $K^{\mathbb{C}}$-orbits of w_1 and w_2 are closed because w_1 and w_2 belong to U_2. Besides, thanks to proposition 3.26, $K^{\mathbb{C}} = N_{G^{\mathbb{C}}}(H^{\mathbb{C}})$. It follows from [29, Corollary 1] that the $G^{\mathbb{C}}$-orbits of w_1 and w_2 are also closed. Since these orbits are constructible, they are Zariski closed (and also $G^{\mathbb{C}}$-stable). Thanks to corollary 3.22, they can be separated by the J_k. This proves our claim.

By Popov & Vinberg's theorem 2.15, the j_k generate the field $(\mathbb{C}(W))^{K^{\mathbb{C}}}$. It follows that the map

$$(\mathbb{C}(V^{\mathbb{C}}))^{G^{\mathbb{C}}} \dashrightarrow (\mathbb{C}(W))^{K^{\mathbb{C}}}$$

is surjective. It remains to go back to real fields of invariants. Thanks to corollary 3.8, we have a diagram

$$\begin{array}{ccc} (\mathbb{C}(V^{\mathbb{C}}))^{G^{\mathbb{C}}} & \dashrightarrow & (\mathbb{C}(W))^{K^{\mathbb{C}}} \\ \| & & \| \\ (\mathbb{C}(V^{\mathbb{C}}))^{G} & \dashrightarrow & (\mathbb{C}(W))^{K} \end{array}$$

Moreover, $\mathbb{C}(V^{\mathbb{C}}) = \mathbb{R}(V) \otimes_{\mathbb{R}} \mathbb{C}$ and $\mathbb{C}(W) = \mathbb{C}((V^H)^{\mathbb{C}}) = \mathbb{R}(V^H) \otimes_{\mathbb{R}} \mathbb{C}$. Hence the map

$$(\mathbb{R}(V))^{G} \dashrightarrow (\mathbb{R}(V^H))^{N_G(H)}$$

is also surjective because every real rational invariant is in the image of a complex rational invariant, and therefore it is also the image of its real part.

We now prove the algebraicity of strata. Thanks to proposition 3.16, there exists a Zariski subset U in $(V^{\mathbb{C}})^{H^{\mathbb{C}}}$ which is contained in the open fixed locus. Let X denotes the $G^{\mathbb{C}}$ orbit of U in $V^{\mathbb{C}}$, then by Chevalley's theorem X is constructible in $V^{\mathbb{C}}$, so its topological closure is the same as its Zariski closure.

Let us first prove that $X \cap V$ lies in Σ_H. If v is in $X \cap V$, then there exists ℓ in $G^{\mathbb{C}}$ such that $\ell \cdot v$ belongs to U. This implies $G^{\mathbb{C}}_{\ell \cdot v} = H^{\mathbb{C}}$, and therefore $\ell\, G^{\mathbb{C}}_v\, \ell^{-1} = H^{\mathbb{C}}$. Since $G^{\mathbb{C}}_v$ and $H^{\mathbb{C}}$ are stable under the Cartan involution ι, we also have $\iota(\ell)\, G^{\mathbb{C}}_v\, \iota(\ell)^{-1} = H^{\mathbb{C}}$. It follows that $\iota(\ell)^{-1}.\ell$ normalizes $G^{\mathbb{C}}_v$. If $\ell = ge^{iZ}$, then $\iota(\ell)^{-1}.\ell = e^{2iZ}$ and thanks to proposition 3.26, Z is in the Lie algebra of $N_G(G_v)$ so e^{iZ} normalizes $G^{\mathbb{C}}_v$. It follows that

$$H^{\mathbb{C}} = ge^{iZ} G^{\mathbb{C}}_v e^{-iZ} g^{-1} = g\, G^{\mathbb{C}}_v\, g^{-1}.$$

Taking the fixed points under the Cartan involution on both sides, $H = g\, G_v\, g^{-1}$, which implies that v lies in the G-orbit of $\overset{\circ}{V}{}^H$.

Let us now prove that $\overline{X \cap V} = \overline{\Sigma}_{[H]}$. The inclusion follows by taking the closure of the inclusion $X \cap V \subset \Sigma_H$. For the other inclusion, recall that U is a Zariski open subset of W and that X is the $G^{\mathbb{C}}$-orbit or U. We have thus $U \cap V^H \subset X \cap V$ and thanks to corollary A.8, $U \cap V^H$ is a nonempty Zariski subset of V^H. Hence, $V^H \subset \overline{X \cap V}$. Since the right hand side is G-stable, we get $\overline{\Sigma}_{[H]} \subset \overline{X \cap V}$.

We can finish the proof as follows: X is Zariski open in $\overline{X}$, so $X \cap V$ is Zariski open in the algebraic set $\overline{X} \cap V$. Therefore, $\overline{X \cap V}$ is also an algebraic set, which is the union of a finite number of irreducible components of $\overline{X} \cap V$. □

Remark 4.1.

- In the first part of the proof, we made crucial use of Luna's criterion for closedness of orbits [29, Corollary 1]. For an easy proof of this theorem using Kempf-Ness theory, see [26].
- The natural candidate for $\overline{\Sigma}_{[H]}$ should be $\overline{X} \cap V$. However, we don't know if $\overline{X} \cap V$ is irreducible in full generality. Hence the best result we could get is that $\overline{\Sigma}_{[H]}$ is one of its irreducible components.

Appendix A. Lie groups and real analytic structures

In this appendix, we recall a few results we need about Lie groups, and add some folklore results on real analytic functions and real analytic manifolds.

We now focus on Lie groups, and recall the following classic formula.

Lemma A.1 (Baker-Campbell-Hausdorff formula)**.** [12, §3.4] *Let G be Lie group and $\mathfrak{g}$ its Lie algebra. Consider $X, Y \in \mathfrak{g}$. Then the solution $Z \in \mathfrak{g}$ of $e^X e^Y = e^Z$ is a formal series in iterated commutators of X and Y*

$$Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] - \frac{1}{12}[Y,[X,Y]] + \cdots,$$

where "$\cdots$" indicates terms involving higher commutators of X and Y. If X and Y are sufficiently small elements of the Lie algebra $\mathfrak{g}$, the series is convergent.

This formula implies that the multiplication of G in exponential coordinates near the neutral element is real analytic. From this, one deduces immediately the following result.

Corollary A.2. *Let G be a Lie group. Then G has a natural real analytic structure such that:*

- *The multiplication map is globally real-analytic*
- *For any g in G the map $L_g \circ \exp$ in a neighborhood of 0 defines a local real analytic chart near g.*

Besides, if H is a Lie subgroup of G, then H is a real analytic submanifold of G. More generally, any continuous morphism between compact Lie groups is real analytic.

Lastly, let us state the following lemma, which is the differentiable version of [38, Proposition 3.7].

Lemma A.3. *Let L be a Lie group with a finite number of connected components, K be a closed subgroup of L, and assume that there exists ℓ in L such that $\ell K \ell^{-1} \subset K$. Then, ℓ normalizes K.*

Proof. The automorphism $\mathrm{Ad}(\ell)$ stabilizes $\mathfrak{k}$, so it is an automorphism of $\mathfrak{k}$. Therefore $\mathrm{Ad}(\ell^{-1})$ stabilizes $\mathfrak{k}$ so $\ell^{-1}K^e\ell \subset K^e$.

Let K/K^e be the set of connected components of K. Then K/K^e is a finite group and $\mathrm{Ad}(\ell)$ induces an action on K/K^e. Let k be a representative of an element of K/K^e which is in the kernel of $\mathrm{Ad}(\ell)$. Then $\ell k \ell^{-1}$ belongs to K^e so $k = \ell^{-1}(\ell\gamma\ell^{-1})\ell \in K^e$, which means that the class of k is 0 in K/K^e. Hence $\mathrm{Ad}(\ell)$ is injective, and since K/K^e is finite, $\mathrm{Ad}(\ell)$ is a bijection. This implies that for any k in K there exists an element of the form $\ell k' \ell^{-1}$ in the connected component of k. This means that there exists k'' in K^e such that $\ell k' \ell^{-1} = k'' k$ so we get $\ell^{-1} k \ell = \ell^{-1}\left((k'')^{-1}\ell k' \ell^{-1}\right)\ell = \left(\ell^{-1}(k'')^{-1}\ell\right)k' \in K$. □

We now recall a folklore results on propagation of local real analytic identities.

Lemma A.4. *Let n be a positive integer, let V be an open and connected subset of $\mathbb{R}^n$, and $f : V \to \mathbb{R}$ a real analytic function. If there exists $v \in V$ such that $f = 0$ on a neighborhood of v then $f = 0$ on V.*

Proof. Let S be the set of points x in U such that all partial derivatives of f vanish at x. This set is closed, but since f is real analytic it is also open. Since $v \in S$, S is nonempty so $S = V$. □

Corollary A.5. *Let n be a positive integer, and assume to be given the following data:*

- *V is an open and connected subset of $\mathbb{R}^n$,*
- *Z is a real analytic manifold,*
- *Y is a (closed) real-analytic submanifold of Z,*
- *$f\colon V \to Z$ is an analytic function.*

Assume that there exists a point v in V and a neighborhood U_v of v in V such that $f(U_v) \subset Y$. Then $f(V) \subset Y$.

Proof. Let W be the subset of points x in V such that there exists a neighborhood U_x of x in V such that $f(U_x) \subset Y$. By definition, W is open. Let x be a point in $\overline{W} \cap V$. As Y is closed, $f(x) \in Y$. Let $\varphi\colon U_y \to \mathbb{R}^m$ be a real analytic chart on a neighborhood U_y of y in Z, such that $U_y \cap Y$ is given by the equations $\varphi_1 = \cdots = \varphi_r = 0$, and let U_x be a connected neighborhood of x in V such that $f(U_x) \subset U_y$. Then, for $1 \leq i$, $\varphi_i \circ f$ is a real analytic function on U_x that vanishes on an open subset of U_x (since $x \in \overline{W}$). By lemma A.4, for $1 \leq i \leq r$, $\varphi_i \circ f$ vanishes in U_x, which means that $f(U_x) \subset Y$, so $x \in W$. It follows that $\overline{W} \cap V = W$, which means that W is closed in V. Since V is connected, $W = V$ and in particular $f(V) \subset Y$. □

We end this appendix with some classical results on totally real submanifolds. Let X be a complex manifold. A real submanifold S of X is *totally real* if for any s in S, $\mathrm{T}_s S$ is a totally real subspace of $\mathrm{T}_s X$, which means that $\mathrm{T}_s S \cap i\mathrm{T}_s S = \{0\}$.

Lemma A.6. *Assume that S is a totally real submanifold of a complex manifold that is moreover real analytic. Then, around each point s of S, there exists an holomorphic chart $\varphi\colon U_s \to \mathbb{C}^n$, where U_s is a neighborhood of s, such that $\varphi(U_s \cap S) = \varphi(U_s) \cap \mathbb{R}^k$.*

Proof. Let $f\colon \mathbb{R}^k \to S$ be a real analytic parametrization of S defined in a neighborhood of 0 such that $f(0) = s$. We can complexify f to a map $F \to \mathbb{C}^k$. Now, for each point z in $\mathbb{C}^k$ near 0, $dF_0(u + iv) = df_0(u) + idf_0(v)$. Since $T_s S$ is totally real, we see that dF_0 is injective and has rank k. It follows that F parameterizes a complex manifold of X containing S. The result follows. □

Corollary A.7. *Let X be a complex manifold and S be a totally real and real analytic submanifold of X of maximal dimension. Then the analytic Zariski closure of S is the union of the connected components of X which intersect S.*

Proof. It is enough to deal with the case where X is connected. Let Z be a complex analytic set containing S. For any point s in S, let Z' be an irreducible component of Z containing s and let us write locally $Z' = \bigcap_{i=1}^r \{f_i = 0\}$ around s. According to lemma A.6, we can write locally the inclusion of S in Z around s as the inclusion of $\mathbb{R}^N$ in $\mathbb{C}^N$ near 0. Then, $f_{i|\mathbb{R}^N} = 0$. Since for any multi-index $I = \{i_1, \ldots, i_N\}$ we have

$$\frac{\partial^I f}{\partial z_I}(0) = \frac{\partial^I f}{\partial x_I}(0) = 0,$$

we see that $f_i = 0$, so Z' contains a neighborhood of s in X. Hence $Z' = X$. □

Corollary A.8. *Let V be a real vector space of finite dimension. If U is a nonempty Zariski open set in $V^{\mathbb{C}}$, then $U \cap V$ is a nonempty Zariski open set in V.*

Proof. Let Z be the complement of U in $V^{\mathbb{C}}$. Then Z is a closed analytic subset of $V^{\mathbb{C}}$. Assume that $U \cap V = \emptyset$. Then Z contains V, so it contains its Zariski closure. Thanks to corollary A.7, $Z = V^{\mathbb{C}}$ so $U = \emptyset$ and we get a contradiction. Hence $U \cap V \neq \emptyset$ and the result follows. □

Appendix B. Proof of the principal orbit theorem in the linear case

In this appendix, we provide for the reader's convenience a proof of theorem 2.6 for the linear case, which combines the ideas of the proofs presented in [10] and [38].

We first need a topological lemma, which allows to propagate connexity.

Lemma B.1. *Let X be a connected topological space, U a dense subset of X, and assume than for any point x in X, there exists a neighborhood U_x of x such that $U \cap U_x$ is connected. Then U is connected.*

Proof. Assume that U can we written as the disjoint union of two nonempty open sets U_1 and U_2. Since U is dense, $X = \overline{U}_1 \cup \overline{U}_2$ and since X is connected, $\overline{U}_1 \cap \overline{U}_2 \neq \emptyset$. Let x in $\overline{U}_1 \cap \overline{U}_2$. Let U_x be a neighborhood of x such that $U \cap U_x$ is connected. Then $U \cap U_x$ is the disjoint union of $U_1 \cap U_x$ and $U_2 \cap U_x$. However these two open sets are non empty, and we get a contradiction. Hence U is connected. □

Remark B.2. This lemma can be better visualized in term of sheaf theory, let $j\colon U \hookrightarrow X$ denote the inclusion, and let us consider the morphism of sheaves $\Delta\colon \mathbb{Z}_X \to j_*\mathbb{Z}_U$. Then the two hypotheses can be translated as follows:

- U is dense in X if and only if Δ is a monomorphism.
- The second property is granted if and only if there exists a covering $(U_i)_{i\in I}$ of U such that Δ_{U_i} is an isomorphism.

We claim that these two properties imply that Δ_X is also an isomorphism. Indeed, the injectivity is straightforward and for the surjectivity, we argue as follows: if s is a global section of $j_*\mathbb{Z}_U$ on X, then for all i, we can write $s_{|U_i} = \Delta_{U_i}(t_i)$, and therefore $\Delta_{U_i\cap U_j}(t_i - t_j) = 0$. Since Δ is a monomorphism, the $(t_i)'s$ glue together to a global section t of $\mathbb{Z}_X$ such that $\Delta_X(t) = s$.

To conclude, we write

$$\mathrm{H}^0(U, \mathbb{Z}_U) = \mathrm{H}^0(X, j_*\mathbb{Z}_U) \simeq \mathrm{H}^0(X, \mathbb{Z}_X) \simeq \mathbb{Z},$$

and therefore U is connected.

Now we explain how to construct linear slices explicitly.

Lemma B.3. *Assume that G acts by orthogonal transformations on V. For any v in V, let E_v be the tangent space of the orbit $G\cdot v$ at v. Then, $E_v^\perp$ is a linear subspace of V, stable by G_v, and meets all G-orbits in V. Besides, a neighborhood of v in $E_v^\perp$ is a local slice of the G-action at v.*

Proof. The Lie algebra $\mathfrak{g}$ of G acts on V, besides this action is given by a morphism from $\mathfrak{g}$ to $\mathfrak{o}(V)$. The tangent space of $G\cdot v$ at v is given by

$$E_v = \{X\cdot v, X \in \mathfrak{g}\}$$

Since X acts by an element of $\mathfrak{o}(V)$, $(X\cdot v|v) = 0$ so v is orthogonal to E_v. Besides, if g is in G_v, w is in $E_v^\perp$ and X is in $\mathfrak{g}$, we have

$$(g\cdot w|X\cdot v) = (w|g^{-1}\cdot(X\cdot v)) = (w|\mathrm{Ad}(g^{-1})(X)\cdot v) = 0$$

so $g\cdot w$ belongs to $E_v^\perp$. Hence $E_v^\perp$ is stable by G_v.

Let $\mathcal{O}$ be an orbit in V, and assume that w is the point of $\mathcal{O}$ that minimizes the distance to v. Then w is a critical point for the function $g \mapsto \|g^{-1}\cdot w - v\|^2 = \|g\cdot v - w\|^2$, which means that for all X in $\mathfrak{g}$, $(X\cdot v|v-w) = 0$. Since v belongs to $E_v^\perp$, so does w. □

Proof of theorem 2.6, linear case. We argue by induction on the dimension on V. The case $V = \{0\}$ is obvious. We now separate two different situations.

Case 1: the representation $\rho\colon \mathfrak{g} \to \mathfrak{o}(V)$ is trivial. Then, the representation itself is trivial on the neutral component of G, which means that G factors to a representation of the finite group G/G^e. Let Γ be the image of the representation, it is a finite group acting faithfully on V. Principal points are exactly the complement of the finite union of the fixed loci V^γ for γ in $\Gamma\setminus\{e\}$. It is open and dense, we denote it by U. Let us now partition $\Gamma\setminus\{e\}$ as $\Gamma_1\cup\Gamma_2$ where

$$\Gamma_1 = \{\gamma\in\Gamma, \operatorname{codim} V^\gamma = 1\}, \quad \text{and} \quad \Gamma_2 = \{\gamma\in\Gamma, \operatorname{codim} V^\gamma \geq 2\}.$$

Let us write $\Gamma_1 = \{\gamma_1,\dots,\gamma_p\}$, $\Gamma_2 = \{\gamma_{p+1},\dots,\gamma_{p+q}\}$, and let us define inductively open subsets $(\Omega_i)_{1\leq i\leq p+q}$ of V as follows: $\Omega_0 = \Omega$ and $\Omega_i = \Omega_{i-1}\cap(V^{\gamma_i})^c$. Then, each Ω_i is dense in Ω_{i-1}. Besides, for any v in $\Omega_{i-1}\cap V^{\gamma_i}$, if B is a small ball centered in v, then we separate two cases.

- If $1\leq i\leq p$, then $B\cap(V^{\gamma_i})^c$ is connected.
- If $p+1\leq i\leq p+q$, $B\cap(V^{\gamma_i})^c$ is not connected because V^{γ_i} is an hyperplane, but γ_i has order 2 in Γ. Hence γ_i swaps the two connected components of $B\cap(V^{\gamma_i})^c$, so $\pi(B\cap(V^{\gamma_i})^c)$ is connected.

Hence it follows by induction using lemma B.1 that all $\pi(\Omega_k)$ are connected. In particular, since $\Omega_{p+q} = U_\Omega = U\cap\Omega$, $\pi(U_\Omega)$ is connected.

Case 2: the representation $\rho\colon \mathfrak{g}\to\mathfrak{o}(V)$ is not trivial. Let

$$W = \{v\in V \text{ such that } \forall X\in\mathfrak{g}, X\cdot v = 0\}$$

be the kernel of the representation ρ. Then, by hypothesis, W is a proper vector subspace of V.

First we claim that W has codimension at least 2. Indeed, if W has codimension 1, then the line $W^\perp$ is stable by the action of G^e. Since orthogonal transformations of a line are ± 1, the action of G^e is trivial on this line, which implies that $W = V$ and gives a contradiction. It follows from this that $\pi(\Omega \cap W^c)$ is connected.

Next we claim that points of W are not principal. Indeed, if w is in W, G_w contains the identity component G^e of G. If w was principal, then for any w' close to w, the same property would hold for $G_{w'}$. This would imply that w' is in W, so W would have nonempty interior. Hence we can replace Ω by $\Omega \cap W^\perp$ without changing the conclusions, that is assume that $\Omega \cap W = \emptyset$.

If v is in Ω, thanks to lemma B.3, we can apply the induction hypothesis with the action of G_v on $E_v^\perp$ which has smaller dimension. Let us consider a small G_v-stable open ball B centered at v in $E_v^\perp$. If the radius is small enough, B is a local slice of the G-action at v. Let $\mathcal{P}$ be the set of principal points in B. By induction, since B is open and connected in $E_v^\perp$, $\mathcal{P}$ is open and dense in B, and $\mathcal{P}/G_v$ is connected.

Let us now remark that since B is a local slice, for any v' in B, $(G_v)_{v'} = G'_v$. It follows that $\mathcal{P}$ consists of principal points of B, but also of V. This proves that v is in the closure of U_Ω, so U_Ω is dense in Ω.

Since B is a local slice, we can assume, up to shrinking B, that the action map $G \times B \to V$ is an open map. Hence, $U_v = G.\mathcal{P}$ is an open subset of principal points in V, and furthermore $U_v/G = \mathcal{P}/G_v$ is connected.

We can now conclude by applying lemma B.1 to the pair $(\pi(U_\Omega), \pi(\Omega))$. For v in Ω, we can consider the neighborhood $G \cdot B$ of v in V. Then $U_\Omega \cap G \cdot B = U_v$ so $\pi(U_\Omega) \cap \pi(G \cdot B) = \mathcal{P}/G_v$ is connected. Hence $\pi(U_\Omega)$ is connected. □

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Chapter 3

O(3) and SO(3)-representations on space of tensors

Any finite-dimensional representation of a compact Lie group has a finite number of isotropy classes. An interesting problem would be to find the isotropy classes of a group representation. In the specific case of the three dimensional group O(3), there exist effective methods to obtain the isotropy classes of irreducible representations, and also of some reducible ones. We extend here such results to all reducible O(3)-representations using clips operation. The calculation done in this chapter is contained in an article accepted for publication in *Mathematics and Mechanics of Complex Systems* ([5]).

Denote by $\mathbb{T}^n(\mathbb{R}^3)$ the vector space of n-th order tensors on the Euclidean space $\mathbb{R}^3$. We consider the representation of the rotation group SO(3) on $\mathbb{T}^n(\mathbb{R}^3)$ given by (using Einstein notation)

$$(\rho_n(g)\mathbf{T})_{i_1\dots i_n} = g_{i_1j_1}g_{i_2j_2}\dots g_{i_nj_n}\mathbf{T}_{j_1\dots j_n}, \quad g \in \mathrm{SO}(3),\ \mathbf{T} \in \mathbb{T}^n(\mathbb{R}^3). \tag{3.1}$$

ρ_n is called the standard representation. Thanks to the Euclidean scalar product on $\mathbb{R}^3$, we do not have to distinguish between covariant and contravariant tensors. As for the full orthogonal group $\mathrm{O}(3) = \mathrm{SO}(3) \oplus \{\pm\mathrm{I}\}$, another representation arises according to the possibility of $-\mathrm{I}$ acting trivially or as minus the identity. When $-\mathrm{I}$ acts trivially, the representation of O(3) on $\mathbb{T}^n(\mathbb{R}^3)$ is reduced to the representation of SO(3) and when $-\mathrm{I}$ acts as minus the identity, we consider the following representation

$$\hat{\rho}_n(g)\mathbf{T} = \det(g)\rho_n(g)\mathbf{T}. \tag{3.2}$$

$\hat{\rho}_n$ is called the twisted representation and such a tensor $\mathbf{T}$ is called a pseudo–tensor.

Note that the representation of even degree ρ_{2p} of O(3) on a tensor space is reduced to the representation of SO(3) ($(\rho_{2n}, \mathrm{O}(3))$ is equivalent to $(\rho_{2n}, \mathrm{SO}(3))$). In this case, the representation of O(3) is only reduced to the twisted representation.

3.1 Closed O(3)-subgroups

In the following, the notation $\mathbf{r}(\boldsymbol{n},\theta)$, with $\theta \in [0;2\pi[$ and $\boldsymbol{n} = (n_x, n_y, n_z)$, a unit vector, denotes the Rodrigues formula to represent a rotation by angle θ around $\boldsymbol{n}$, which is given by

$$\mathbf{r}(\boldsymbol{n},\theta) = \exp(\theta j(\boldsymbol{n})) = \mathrm{I} + j(\boldsymbol{n})\sin(\theta) + j(\boldsymbol{n})^2(1-\cos(\theta))$$

where $j(\boldsymbol{n})$ denotes the antisymmetric matrix with entries

$$j(\boldsymbol{n}) = \begin{pmatrix} 0 & -n_z & n_y \\ n_z & 0 & -n_x \\ -n_y & n_x & 0 \end{pmatrix}.$$

Given a subgroup Γ of O(3), set

$$\Gamma_+ = \{g \in \Gamma \ \mid \ \det g = 1\} \text{ and } \Gamma_- = \{g \in \Gamma \ \mid \ \det g = -1\}.$$

Then $\Gamma = \Gamma_+ \cup \Gamma_-$ and we have the following classification (see [43, chapter XIII section 9], [19, page 352]).

Type I: A closed subgroup Γ of O(3) is of type I if $\Gamma_- = \emptyset$, in which case Γ is a subgroup of SO(3). A subgroup of type I is conjugate to one of the following list

$$\mathrm{SO}(3), \quad \mathrm{O}(2), \quad \mathrm{SO}(2), \quad \mathbb{D}_n, \quad \mathbb{Z}_n, \quad \mathbb{T}, \quad \mathbb{O}, \quad \mathbb{I}, \text{ or } \mathbb{1}$$

Type II: A closed subgroup Γ of O(3) is of type II if $-\mathrm{I} \in \Gamma$, in which case $-\Gamma_- = \Gamma_+$ and $\Gamma = \Gamma_+ \cup -\Gamma_+$. A subgroup of type II is a direct product of a subgroup of type I and the subgroup $\mathbb{Z}_2^c = \{\pm\mathrm{I}\}$, it is a conjugate to one in the following list

$$\mathrm{SO}(3)\oplus\mathbb{Z}_2^c, \quad \mathrm{O}(2)\oplus\mathbb{Z}_2^c, \quad \mathrm{SO}(2)\oplus\mathbb{Z}_2^c, \quad \mathbb{Z}_m\oplus\mathbb{Z}_2^c, \quad \mathbb{D}_m\oplus\mathbb{Z}_2^c, \quad \mathbb{T}\oplus\mathbb{Z}_2^c, \quad \mathbb{O}\oplus\mathbb{Z}_2^c, \quad \mathbb{I}\oplus\mathbb{Z}_2^c$$

Type III: A closed subgroup Γ of O(3) is of type III if $\Gamma_- \neq \emptyset$ but $-\mathrm{I} \notin \Gamma$. Then, Γ_+ is a subgroup of index 2 in the subgroup $\tilde{\Gamma} = \Gamma_+ \cup (-\Gamma_-)$ of SO(3). In that case, there exists $\gamma \in \tilde{\Gamma} \setminus \Gamma_+$ such that $-\Gamma_- = \gamma\Gamma_+$ and $\Gamma = \Gamma_+ \cup -\gamma\Gamma_+$. Five representatives of conjugacy classes of subgroups of type III can be deduced

$$\mathbb{Z}_{2n}^- = \mathbb{Z}_n \cup (-\mathbf{r}(\boldsymbol{e}_3, \frac{\pi}{n}))\mathbb{Z}_n \quad \forall n \geq 1. \tag{3.3}$$

$$\mathbb{D}_n^z = \mathbb{Z}_n \cup (-\mathbf{r}(\boldsymbol{e}_1, \pi))\mathbb{Z}_n \quad \forall n \geq 2. \tag{3.4}$$

$$\mathbb{D}_{2n}^d = \mathbb{D}_n \cup (-\mathbf{r}(\boldsymbol{e}_3, \frac{\pi}{n}))\mathbb{D}_n \quad \forall n \geq 1. \tag{3.5}$$

$$\mathbb{O}^- = \mathbb{T} \cup (-\mathbf{r}(\boldsymbol{e}_3, \frac{\pi}{2}))\mathbb{T}. \tag{3.6}$$

$$\mathrm{O}(2)^- = \mathrm{SO}(2) \cup (-\mathbf{r}(\boldsymbol{e}_1, \pi))\mathrm{SO}(2). \tag{3.7}$$

In figure 3.1, conjugacy classes of closed SO(3)-subgroups are represented. An arrow from a class $[H_1]$ to a class $[H_2]$ means that $[H_1] \preceq [H_2]$ where $\preceq$ is the partial relation order on

the set of conjugacy classes defined in theorem 1.2.9. Relations between conjugacy classes of O(3)-subgroups can be found in [19, table A.5].

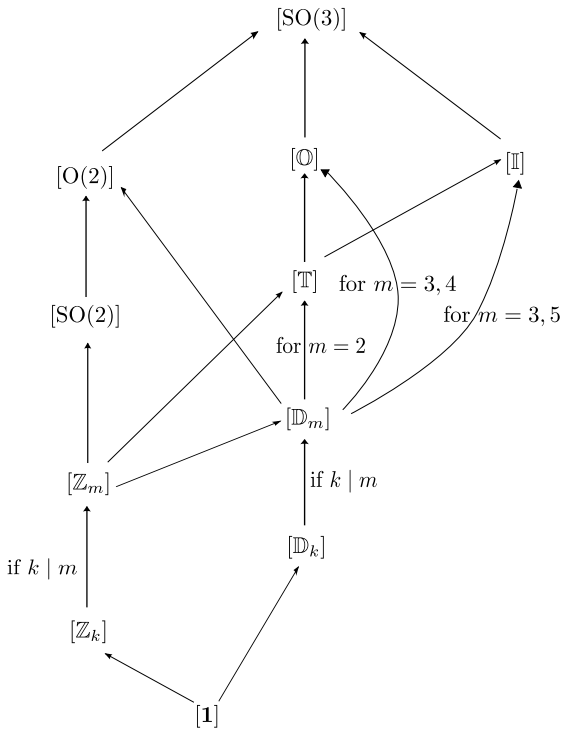

Figure 3.1: Diagram of SO(3)-subgroups.

Example 3.1.1. *Consider the example of $\mathbb{Z}_4^-$ (a type III* O(3)*-subgroup) deduced using $\mathbb{Z}_2$ and $\mathbf{r}(\boldsymbol{e}_3, \pi/2)$ as in equation (3.3) above:*

$$\mathbb{Z}_4^- = \mathbb{Z}_2 \cup (-\mathbf{r}(\boldsymbol{e}_3, \pi/2)\mathbb{Z}_2) = \{\mathrm{I}, \mathbf{r}(\boldsymbol{e}_3, \pi), -\mathbf{r}(\boldsymbol{e}_3, \pi/2), -\mathbf{r}(\boldsymbol{e}_3, 3\pi/2)\}\,.$$

We propose, in Table 3.1, generators for type I and type III closed O(3)-subgroups.

We give now some useful decomposition of subgroups $\mathbb{T}, \mathbb{O}$ and $\mathbb{I}$. To do so, let us first introduce the subgroup

$$\mathbb{Z}_n^{\boldsymbol{u}} := \left\langle \mathbf{r}\left(\boldsymbol{u}, \frac{2\pi}{n}\right)\right\rangle, \tag{3.8}$$

where the axis $\langle \boldsymbol{u} \rangle$ generated by $\boldsymbol{u}$ is said to be the primary axis of $\mathbb{Z}_n^{\boldsymbol{u}}$. We have

$$\mathbb{Z}_n = \mathbb{Z}_n^{\boldsymbol{e}_3}$$

and, for any $g \in \mathrm{SO}(3)$,

$$g\mathbb{Z}_n g^{-1} = \mathbb{Z}_n^{g\boldsymbol{e}_3}.$$

In particular, $\mathbb{Z}_n$ is given by

$$\mathbb{Z}_n = \left\{\mathbf{r}\left(\boldsymbol{e}_3, \frac{2k\pi}{n}\right), k = 0, \ldots, n-1\right\}, \tag{3.9}$$

Type I subgroup	Order	Generators
$\mathbb{Z}_n,\ n \geq 2$	n	$\mathbf{r}\left(\boldsymbol{e}_3, {}^{2\pi}/_{n}\right)$
$\mathbb{D}_n,\ n \geq 2$	$2n$	$\mathbf{r}\left(\boldsymbol{e}_3, {}^{2\pi}/_{n}\right),\ \mathbf{r}(\boldsymbol{e}_1, \pi)$
$\mathbb{T}$	12	$\mathbf{r}(\boldsymbol{e}_3, \pi),\ \mathbf{r}(\boldsymbol{e}_1, \pi),\ \mathbf{r}(\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3, {}^{2\pi}/_{3})$
$\mathbb{O}$	24	$\mathbf{r}(\boldsymbol{e}_3, {}^{\pi}/_{2}),\ \mathbf{r}(\boldsymbol{e}_1, \pi),\ \mathbf{r}(\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3, {}^{2\pi}/_{3})$
$\mathbb{I}$	60	$\mathbf{r}(\boldsymbol{e}_3, \pi),\ \mathbf{r}(\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3, {}^{2\pi}/_{3}), \mathbf{r}(\boldsymbol{e}_1 + \phi\boldsymbol{e}_3, {}^{2\pi}/_{5}) \quad \phi := (1+\sqrt{5})/2$
SO(2)	∞	$\mathbf{r}(\boldsymbol{e}_3, \theta), \quad \theta \in [0, 2\pi]$
O(2)	∞	$\mathrm{SO}(2), \mathbf{r}(\boldsymbol{e}_1, \pi)$
Type III subgroup		
$\mathbb{Z}_2^-$	2	$-\mathbf{r}(\boldsymbol{e}_3, \pi)$
$\mathbb{Z}_{2n}^-,\ n \geq 2$	$2n$	$-\mathbf{r}\left(\boldsymbol{e}_3, {}^{\pi}/_{n}\right)$
$\mathbb{D}_{2n}^d,\ n \geq 2$	$4n$	$-\mathbf{r}\left(\boldsymbol{e}_3, {}^{\pi}/_{n}\right),\ \mathbf{r}(\boldsymbol{e}_1, \pi)$
$\mathbb{D}_n^z,\ n \geq 2$	$2n$	$\mathbf{r}\left(\boldsymbol{e}_3, {}^{2\pi}/_{n}\right),\ -\mathbf{r}(\boldsymbol{e}_1, \pi)$
$\mathbb{O}^-$	24	$-\mathbf{r}(\boldsymbol{e}_3, {}^{\pi}/_{2}),\ -\mathbf{r}(\boldsymbol{e}_2 - \boldsymbol{e}_3, \pi)$
$\mathrm{O}(2)^-$	∞	$\mathrm{SO}(2), -\mathbf{r}(\boldsymbol{e}_1, \pi)$

Table 3.1: Generators of closed O(3)-subgroups

and $\mathbb{D}_n$ by

$$\mathbb{D}_n = \left\{\mathbf{r}\left(\boldsymbol{e}_3, \frac{2k\pi}{n}\right), \mathbf{r}(\mathbf{b}_i, \pi); \quad k = 0, \ldots, n-1,\ i = 1, \ldots, n\right\}, \tag{3.10}$$

with $\mathbf{b}_i$ being the secondary axis of $\mathbb{D}_n$ in the (xy)-plane such that $\mathbf{b}_1 = \boldsymbol{e}_1$ and $\mathbf{b}_i = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{n}\right)\mathbf{b}_{i-1}$ for $i \geq 2$. We propose now details on compositions of the subgroups $\mathbb{T}$, $\mathbb{O}$ and $\mathbb{I}$, with explicit axes for all cyclic and dihedral subgroups they contain.

First, we have (see [53] for instance)

$$\mathbb{T} = \bigcup_{i=1}^{3} \mathbb{Z}_2^{\boldsymbol{e}_i} \cup \bigcup_{j=1}^{4} \mathbb{Z}_3^{\boldsymbol{s}_{t_j}} \tag{3.11}$$

with

$$\boldsymbol{s}_{t_1} = \boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3, \quad \boldsymbol{s}_{t_2} = \boldsymbol{e}_1 - \boldsymbol{e}_2 - \boldsymbol{e}_3, \quad \boldsymbol{s}_{t_3} = -\boldsymbol{e}_1 + \boldsymbol{e}_2 - \boldsymbol{e}_3, \quad \boldsymbol{s}_{t_4} = -\boldsymbol{e}_1 - \boldsymbol{e}_2 + \boldsymbol{e}_3.$$

For the cubic group, we have

$$\mathbb{O} = \bigcup_{i=1}^{3} \mathbb{Z}_4^{\boldsymbol{e}_i} \cup \bigcup_{j=1}^{4} \mathbb{Z}_3^{\boldsymbol{s}_{t_j}} \cup \bigcup_{k=1}^{6} \mathbb{Z}_2^{\boldsymbol{a}_{c_k}} \tag{3.12}$$

with vectors $\mathbf{a}_k$ given by

$$\begin{aligned} &\mathbf{a}_{c_1} = \mathbf{e}_1 + \mathbf{e}_2, \quad \mathbf{a}_{c_2} = \mathbf{e}_1 - \mathbf{e}_2, \quad \mathbf{a}_{c_3} = \mathbf{e}_1 + \mathbf{e}_3 \\ &\mathbf{a}_{c_4} = \mathbf{e}_1 - \mathbf{e}_3, \quad \mathbf{a}_{c_5} = \mathbf{e}_2 + \mathbf{e}_3, \quad \mathbf{a}_{c_6} = \mathbf{e}_2 - \mathbf{e}_3. \end{aligned} \tag{3.13}$$

Finally, we have

$$\mathbb{I} = \bigcup_{i=1}^{6} \mathbb{Z}_5^{\boldsymbol{u}_i} \cup \bigcup_{j=1}^{10} \mathbb{Z}_3^{\boldsymbol{v}_j} \cup \bigcup_{k=1}^{15} \mathbb{Z}_2^{\boldsymbol{w}_k} \tag{3.14}$$

Taking $\phi := \frac{(1+\sqrt{5})}{5}$ to be the golden ratio, vectors $\boldsymbol{u}_i$ are obtained as centers of icosahedron faces ([86, Figure 11]):

$$\begin{aligned} &\boldsymbol{u}_1 := (1+3\phi)\boldsymbol{e}_1 + (2+\phi)\boldsymbol{e}_3, \quad \boldsymbol{u}_2 := (2+\phi)\boldsymbol{e}_1 + (1+3\phi)\boldsymbol{e}_2, \quad \boldsymbol{u}_3 := (2+\phi)\boldsymbol{e}_2 - (1+3\phi)\boldsymbol{e}_3 \\ &\boldsymbol{u}_4 := -(2+\phi)\boldsymbol{e}_2 - (1+3\phi)\boldsymbol{e}_3, \quad \boldsymbol{u}_5 = (1+3\phi)\boldsymbol{e}_1 - (2+\phi)\boldsymbol{e}_3, \quad \boldsymbol{u}_6 := (2+\phi)\boldsymbol{e}_1 - (1+3\phi)\boldsymbol{e}_2. \end{aligned}$$

Then vectors $\boldsymbol{v}_j$ are obtained from vertices of icosahedron:

$$\begin{aligned} &\boldsymbol{v}_1 := \boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3, \quad \boldsymbol{v}_2 := \phi\boldsymbol{e}_1 + \frac{1}{\phi}\boldsymbol{e}_2, \quad \boldsymbol{v}_3 := \boldsymbol{e}_1 + \boldsymbol{e}_2 - \boldsymbol{e}_3, \quad \boldsymbol{v}_4 := \phi\boldsymbol{e}_2 - \frac{1}{\phi}\boldsymbol{e}_3 \\ &\boldsymbol{v}_5 := \phi\boldsymbol{e}_2 + \frac{1}{\phi}\boldsymbol{e}_3, \quad \boldsymbol{v}_6 := -\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3, \quad \boldsymbol{v}_7 := -\phi\boldsymbol{e}_1 + \frac{1}{\phi}\boldsymbol{e}_2, \quad \boldsymbol{v}_8 := -\boldsymbol{e}_1 + \boldsymbol{e}_2 - \boldsymbol{e}_3 \\ &\boldsymbol{v}_9 := -\frac{1}{\phi}\boldsymbol{e}_1 - \phi\boldsymbol{e}_3, \quad \boldsymbol{v}_{10} := \frac{1}{\phi}\boldsymbol{e}_1 - \phi\boldsymbol{e}_3 \end{aligned}$$

while vectors $\boldsymbol{w}_k$ are obtained from its edges:

$$\begin{aligned} &\boldsymbol{w}_1 := \boldsymbol{e}_1 + (\phi+1)\boldsymbol{e}_2 + \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_3, \quad \boldsymbol{w}_2 := \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_1 + \boldsymbol{e}_2 + (\phi+1)\boldsymbol{e}_3 \\ &\boldsymbol{w}_3 := (\phi+1)\boldsymbol{e}_1 + \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_2 + \boldsymbol{e}_3, \quad \boldsymbol{w}_4 := \phi\boldsymbol{e}_1, \quad \boldsymbol{w}_5 := (\phi+1)\boldsymbol{e}_1 + \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_2 - \boldsymbol{e}_3 \\ &\boldsymbol{w}_6 := (\phi+1)\boldsymbol{e}_1 - \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_2 + \boldsymbol{e}_3, \quad \boldsymbol{w}_7 := \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_1 - \boldsymbol{e}_2 + (\phi+1)\boldsymbol{e}_3, \\ &\boldsymbol{w}_8 := (\phi+1)\boldsymbol{e}_1 - \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_2 - \boldsymbol{e}_3, \quad \boldsymbol{w}_9 := \boldsymbol{e}_1 + (\phi+1)\boldsymbol{e}_2 - \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_3 \\ &\boldsymbol{w}_{10} := \phi\boldsymbol{e}_2, \quad \boldsymbol{w}_{11} := -\boldsymbol{e}_1 + (\phi+1)\boldsymbol{e}_2 + \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_3, \quad \boldsymbol{w}_{12} = \phi\boldsymbol{e}_3 \\ &\boldsymbol{w}_{13} := -\left(1+\frac{1}{\phi}\right)\boldsymbol{e}_1 + \boldsymbol{e}_2 + (\phi+1)\boldsymbol{e}_3, \quad \boldsymbol{w}_{14} := -\boldsymbol{e}_1 + (\phi+1)\boldsymbol{e}_2 - \left(1+\frac{1}{\phi}\right)\boldsymbol{e}_3, \\ &\boldsymbol{w}_{15} := -\left(1+\frac{1}{\phi}\right)\boldsymbol{e}_1 - \boldsymbol{e}_2 + (\phi+1)\boldsymbol{e}_3. \end{aligned}$$

Finally, the subgroups SO(2) and O(2) are given by

$$\mathrm{SO}(2) = \{\mathbf{r}(\boldsymbol{e}_3, \theta), \theta \in [0, 2\pi]\} \tag{3.15}$$

and

$$\mathrm{O}(2) = \{\mathbf{r}(\boldsymbol{e}_3, \theta), \mathbf{r}(\mathbf{b}, \pi),\ \theta \in [0, 2\pi],\ \mathbf{b} \in (xy) - \text{plane}\}\,. \tag{3.16}$$

3.2 Irreducible representations

The study of a representation of a compact Lie group is often made easier by considering its decomposition into a direct sum of irreducible representations (the notion of reducibility is introduced in section 1.2). In fact, any representation of a compact Lie group can be decomposed, non uniquely, into a direct sum of irreducible representations (proof can be found in [43, Chapter XII, section 2]). The irreducible representations of the groups SO(3) and O(3) are known (up to isomorphism). Explicit models for these irreducible representations are provided by the so-called harmonic tensor spaces, described below.

3.2.1 Harmonic tensors

Let $\mathbb{S}^n(\mathbb{R}^3)$ be the subspace of totally symmetric tensors of order n[1]. Contracting two indices i, j on a totally symmetric tensor $\mathbf{S}$ does not depend on the particular choice of the pair (i, j). Thus, we can refer to this contraction without any reference to a particular choice of indices. We will denote this contraction as $\mathrm{tr}(\mathbf{S})$, which is a totally symmetric tensor of order $n-2$ and is called the trace of $\mathbf{S}$.

Definition 3.2.1. *Let $\mathbf{S} \in \mathbb{S}^n(\mathbb{R}^3)$, $\mathbf{S}$ is called* harmonic *if $\mathrm{tr}(\mathbf{S}) = 0$. The space of n-th order harmonic tensors is denoted by $\mathbb{H}^n(\mathbb{R}^3)$ (or simply $\mathbb{H}^n$). $\mathbb{H}^n$ is a linear subspace of $\mathbb{S}^n(\mathbb{R}^3)$ of dimension $2n+1$.*

Remark 3.2.2. *A n-th order tensor $\mathbf{T} \in \mathbb{T}^n(\mathbb{R}^3)$ is a n-linear mapping*

$$\begin{aligned} \mathbf{T}:\ \mathbb{R}^3 \times \mathbb{R}^3 \times \ldots \times \mathbb{R}^3 &\to \mathbb{R} \\ (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) &\mapsto \mathbf{T}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n). \end{aligned}$$

Thus, the subspace $\mathbb{S}^n(\mathbb{R}^3)$ of totally symmetric tensors can be identified with the vector space $\mathcal{P}_n(\mathbb{R}^3)$ of homogeneous polynomials of degree n. Following this correspondence, a traceless totally symmetric tensor $\mathbf{H}$ corresponds to an harmonic polynomial h i.e. with vanishing Laplacian: $\Delta h = 0$. We denote by $\mathcal{H}_n(\mathbb{R}^3)$ the space of harmonic polynomials of degree n. An action of SO(3) *(or* O(3)*) on $\mathcal{H}_n(\mathbb{R}^3)$ is induced by the natural action on $\mathbb{R}^3$:*

$$\textit{for } p \in \mathcal{H}_n(\mathbb{R}^3) \textit{ and } g \in \mathrm{O}(3), \quad (\rho_n(g)p)(\boldsymbol{x}) = p(g^{-1}\boldsymbol{x}).$$

The subspace $\mathbb{H}^n(\mathbb{R}^3)$ is invariant under the action of SO(3) (a rotated harmonic tensor

[1] A tensor of order n is a n-linear map between vector spaces, denoted by n indices. A tensor of order n is totally symmetric if it is invariant under permutation of its n indices.

stays harmonic) and this follows from the fact that the space of harmonic polynomials $\mathcal{H}_n$ is SO(3)-invariant (see [14, proposition 5.10]).

Theorem 3.2.3. *[43, 14] The subspace $\mathbb{H}^n(\mathbb{R}^3)$ is irreducible for the SO(3)-representation ρ_n. Moreover, every irreducible representation of SO(3) is equivalent to $(\mathbb{H}^n(\mathbb{R}^3), \rho_n)$ for some integer n.*

Remark 3.2.4. *Two representations (V, ρ_1) and (W, ρ_2) of a group G are said to be equivalent if there exists an equivariant (definition 1.1.9) linear bijective map from V into W (see [14, definition 1.4]).*

Corollary 3.2.5. *(Harmonic decomposition) Every finite dimensional representation V of the rotation group SO(3) splits into a direct sum of irreducible representations, each of them being isomorphic to an harmonic tensor space $\mathbb{H}^n(\mathbb{R}^3)$.*

As a consequence, we can deduce a similar result for O(3)-representation. Denote by $\mathbb{H}^{\#n}(\mathbb{R}^3)$ the space of harmonic tensors of order n endowed with the twisted representation $\hat{\rho}_n$ defined in (3.2).

Corollary 3.2.6. *[85, corollary 3.1.2] The subspaces $\mathbb{H}^n(\mathbb{R}^3)$ and $\mathbb{H}^{\#n}(\mathbb{R}^3)$ are irreducible for the O(3)-representation. Moreover, every irreducible representation of O(3) is equivalent to $(\mathbb{H}^n(\mathbb{R}^3), \rho_n)$ or $(\mathbb{H}^{\#n}(\mathbb{R}^3), \hat{\rho}_n)$ for some integer n.*

3.2.2 Isotropy classes for irreducible representations

The problem of finding isotropy classes for irreducible representations started in mechanics with the study of symmetry changes of a material, in the sixties. Thereafter, Michel [77, 78] and Sattinger [8] developed a new approach to solve the problem, in the specific case of SO(3)-representations, using a convenient group-theoretic framework. Since then, several contributions have been made in this subject and been extended to O(3)-representations, especially from the mathematical point of view by Ihrig and Gobulitsky [53], and Chossat et al [19] who made several corrections on the results of [53]. In figures 3.2, 3.3 and 3.4, we give the isotropy classes for SO(3)-representation ρ_n on the irreducible spaces $\mathbb{H}^n(\mathbb{R}^3)$, for $n = 3, 4, 5$ deduced from [53, theorem 6.6]. For the case $n = 3$, an error in [53] has been corrected by Olive et al. in [92]. In fact, in [53, theorem 6.6], $[\mathbb{D}_2]$ is said to be an isotropy class for SO(3)-representation on $\mathbb{H}^3(\mathbb{R}^3)$ which is not true.

3.2.3 Characterization of the closed isotropy strata for $\mathbb{H}^4(\mathbb{R}^3)$

In this section, we give a polynomial characterization of the closed isotropy strata of SO(3)-representation ρ_n on the space of harmonic tensors of order 4. For this, we introduce the following symmetric second-order tensors $\mathbf{d}_2, \ldots, \mathbf{d}_{10}$, for $H \in \mathbb{H}^4(\mathbb{R}^3)$:

$$\begin{array}{lll} \mathbf{d}_2 = \mathrm{tr}_{13}(\mathbf{H}^2) & \mathbf{d}_3 = \mathrm{tr}_{13}(\mathbf{H}^3) & \mathbf{d}_4 = \mathbf{d}_2^2 \\ \mathbf{d}_5 = \mathbf{d}_2\mathbf{H}\mathbf{d}_2 & \mathbf{d}_6 = \mathbf{d}_2^3 & \mathbf{d}_7 = \mathbf{d}_2^2\mathbf{H}\mathbf{d}_2 \\ \mathbf{d}_8 = \mathbf{d}_2^2\mathbf{H}^2\mathbf{d}_2 & \mathbf{d}_9 = \mathbf{d}_2^2\mathbf{H}\mathbf{d}_2^2 & \mathbf{d}_{10} = \mathbf{d}_2^2\mathbf{H}^2\mathbf{d}_2^2 \end{array} \tag{3.17}$$

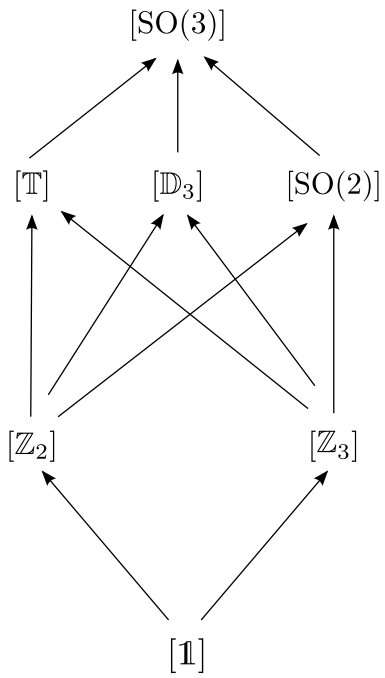

Figure 3.2: The poset of symmetry classes for $\mathbb{H}^3$.

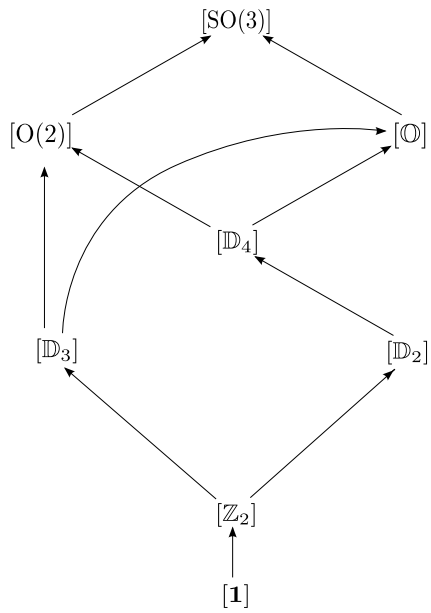

Figure 3.3: The poset of symmetry classes for $\mathbb{H}^4$.

We consider as well the nine fundamental invariants:

$$J_k := \mathrm{tr}(\mathbf{d}_k), \qquad k = 2, \ldots, 10.$$

Denote by $\mathbf{q}$ the euclidean metric and $\boldsymbol{\varepsilon}$ the Levi-Civita tensor. We define the symmetric second-order tensors

$$\mathbf{d}_2' := \mathbf{d}_2 - \frac{1}{3}\,\mathrm{tr}(\mathbf{d}_2)\mathbf{q},\ \mathbf{c}_3 := \mathbf{H} : \mathbf{d}_2,\ \mathbf{c}_4 := \mathbf{H} : \mathbf{c}_3,\ \mathbf{v}_5 := \boldsymbol{\varepsilon} : (\mathbf{d}_2\mathbf{c}_3),\ \mathbf{v}_6 := \boldsymbol{\varepsilon} : (\mathbf{d}_2\mathbf{c}_4).$$

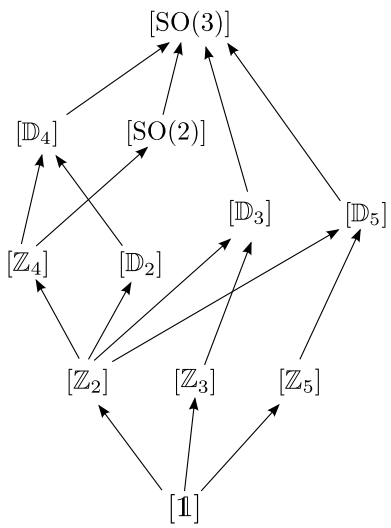

Figure 3.4: The poset of symmetry classes for $\mathbb{H}^5$.

Theorem 3.2.7. *Let* $\mathbf{H} \in \mathbb{H}^4(\mathbb{R}^3)$ *a fourth order harmonic tensor. Then*

(1) $\mathbf{H} \in \overline{\Sigma}_{[\mathrm{SO}(3)]} \iff \mathbf{d}_2' = 0.$

(2) $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{O}]} \iff \mathbf{d}_2' = 0.$

(3) $\mathbf{H} \in \overline{\Sigma}_{[\mathrm{O}(2)]} \iff \mathbf{d}_2 \times \mathbf{d}_2^2 = 0,\ \mathbf{H} \times \mathbf{d}_2 = 0$ *and* $3430 J_3^2 - 81 J_2^3 = 0.$

(4) $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{D}_4]} \iff \mathbf{d}_2 \times \mathbf{d}_2^2 = 0$ *and* $\mathrm{tr}(\mathbf{H} \times \mathbf{d}_2) = 0.$

(5) $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{D}_3]} \iff \mathbf{d}_2 \times \mathbf{d}_2^2 = 0,\ (\mathbf{H} : \mathbf{d}_2) \times \mathbf{d}_2 = 0$ *and* $196 J_6 - 51 J_2^3 + 216 J_2 J_4 + 10 J_3^2 = 0.$

(6) $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{D}_2]} \iff \mathbf{v}_5 = \mathbf{v}_6 = 0,\ \mathrm{tr}(\mathbf{d}_2 \times \mathbf{c}_3) = 0$ *and* $3 J_4 - J_2^2 = 0.$

(7) $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{Z}_2]} \iff \mathbf{v}_5 \times [(\mathbf{v}_5.\mathbf{H}.\mathbf{v}_5)\mathbf{v}_5] = 0$ *and* $\mathbf{v}_5 \times [(\mathbf{v}_5.\mathbf{H}^2.\mathbf{v}_5)\mathbf{v}_5] = 0.$

Proof.

1. For the proof of (*1*) and (*2*) see [91, theorem 9.3].

2. The first implication is deduced from [91, corollary 9.6 & theorem 8.5] together with [2, proposition 4.5]. Conversely, $\mathbf{H}$ belongs to $\overline{\Sigma}_{[\mathrm{O}(2)]}$ (*i.e.* $\mathbf{H}$ is at least transversely isotropic) if $\mathbf{H} \in \Sigma_{[\mathrm{O}(2)]}$ or $\mathbf{H} \in \Sigma_{[\mathrm{SO}(3)]}$. By [91, lemma 8.1], $\mathbf{d}_2 \times \mathbf{d}_2^2 = 0$ imply that $\mathbf{d}_2$ is at least transversely isotropic, which leads to two cases:

   - if $\mathbf{d}_2$ is transversely isotropic then $\mathbf{H} \in \Sigma_{\mathrm{O}(2)}$ since $H \times \mathbf{d}_2 = 0$ [91, corollary 9.6]
   - if $\mathbf{d}_2$ is isotropic (*i.e.* $\mathbf{d}_2' = 0$) then $\mathbf{H} \in \Sigma_{[\mathrm{SO}(3)]}$ or $\mathbf{H} \in \Sigma_{[\mathbb{O}]}$ (by (*1*) and (*2*)). However, the case $\mathbf{H} \in \Sigma_{[\mathbb{O}]}$ is impossible thanks to the equation $3430 J_3^2 - 81 J_2^3 = 0$ [2, proposition 4.5].

   Hence, $\mathbf{H} \in \overline{\Sigma}_{[\mathrm{O}(2)]}$ in all cases.

3. If $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{D}_4]}$ then $\mathbf{H} \in \Sigma_{[\mathbb{D}_4]}$ or $\mathbf{H} \in \Sigma_{[\mathrm{O}(2)]}$ or $\mathbf{H} \in \Sigma_{[\mathbb{O}]}$ or $\mathbf{H} \in \Sigma_{[\mathrm{SO}(3)]}$ (see figure 3.3). If $\mathbf{H} \in \Sigma_{[\mathbb{D}_4]}$ then $\mathbf{d}_2 \in \Sigma_{[\mathrm{O}(2)]}$, $\mathbf{H} \times \mathbf{d}_2 \neq 0$ and $\mathrm{tr}(\mathbf{H} \times \mathbf{d}_2) = 0$ ([91, corollary 9.6]) and by [91, theorem 8.5] $\mathbf{d}_2 \in \Sigma_{[\mathrm{O}(2)]}$ gives the equation $\mathbf{d}_2 \times \mathbf{d}_2^2 = 0$.

   Conversely, suppose that $\mathbf{d}_2 \times \mathbf{d}_2^2 = 0$ and $\mathrm{tr}(\mathbf{H} \times \mathbf{d}_2) = 0$. The equation $\mathbf{d}_2 \times \mathbf{d}_2^2 = 0$ implies that $\mathbf{d}_2$ is either isotropic or transversely isotropic [91, lemma 8.1]:

- if $\mathbf{d}_2$ is isotropic then $\mathbf{d}_2' = 0$ and $H \in \Sigma_{[\mathrm{SO}(3)]} \subset \overline{\Sigma}_{[\mathbb{D}_4]}$,
- if $\mathbf{d}_2$ is transversely isotropic then we consider two cases: if $\mathbf{H} \times \mathbf{d}_2 \neq 0$ then $\mathbf{H} \in \Sigma_{[\mathbb{D}_4]} \subset \overline{\Sigma}_{[\mathbb{D}_4]}$ since $\mathrm{tr}(\mathbf{H} \times \mathbf{d}_2) = 0$. And if $\mathbf{H} \times \mathbf{d}_2 = 0$ then $\mathbf{H} \in \Sigma_{[\mathrm{O}(2)]} \subset \overline{\Sigma}_{[\mathbb{D}_4]}$ [91, corollary 9.6].

4. If $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{D}_3]}$ then $\mathbf{H} \in \Sigma_{[\mathbb{D}_3]}$ and hence $\mathbf{d}_2 \in \Sigma_{\mathrm{O}(2)}$, $\mathrm{tr}(\mathbf{H} \times \mathbf{d}_2) \neq 0$ and $(\mathbf{H} : \mathbf{d}_2) \times \mathbf{d}_2 = 0$ by [91, corollary 9.6]. By [91, theorem 8.5], $\mathbf{d}_2 \in \Sigma_{[\mathrm{O}(2)]}$ gives the equation $\mathbf{d}_2 \times \mathbf{d}_2^2 = 0$. As for the last equation, it is deduced from [2, proposition 4.3].

   Conversely, if $\mathbf{d}_2 \times \mathbf{d}_2^2 = 0$ then $\mathbf{d}_2$ is either isotropic or transversely isotropic [91, lemma 8.1]. If $\mathbf{d}_2$ is isotropic then $H \in \Sigma_{[\mathrm{SO}(3)]} \subset \overline{\Sigma}_{[\mathbb{D}_3]}$ (see figure 3.3). If $\mathbf{d}_2$ is transversely isotropic then we consider two cases:

   - if $\mathrm{tr}(\mathbf{H} \times \mathbf{d}_2) \neq 0$ then $\mathbf{H} \in \Sigma_{[\mathbb{D}_3]} \subset \overline{\Sigma}_{[\mathbb{D}_3]}$ since $(\mathbf{H} : \mathbf{d}_2) \times \mathbf{d}_2 = 0$ [91, corollary 9.6].
   - if $\mathrm{tr}(\mathbf{H} \times \mathbf{d}_2) = 0$ then
     - if $\mathbf{H} \times \mathbf{d}_2 = 0$ then $\mathbf{H} \in \Sigma_{[\mathrm{O}(2)]} \subset \overline{\Sigma}_{[\mathbb{D}_3]}$
     - if $\mathbf{H} \times \mathbf{d}_2 \neq 0$ then $\mathbf{H} \in \Sigma_{[\mathbb{D}_4]}$. However, if $\mathbf{H} \in \Sigma_{[\mathbb{D}_4]} \subset \overline{\Sigma}_{[\mathbb{D}_4]}$ then, using [2, proposition 4.9], $6J_6 = -3J_2^3 + 9J_2J_4 + 20J_3^2$ together with the hypothesis equation $196J_6 - 51J_2^3 + 216J_2J_4 + 10J_3^2 = 0$ will give the following equation $5J_2^3 - 8J_2J_4 - 70J_3^2 = 0$ which contradicts the fact that $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{D}_4]}$.

5. Using [91, theorem 9.10, corollary 8.4] we deduce the first implication.

   Conversely, $\mathbf{v}_5 = \mathbf{v}_6 = 0$ and $\mathrm{tr}(\mathbf{d}_2 \times \mathbf{c}_3) = 0$ imply that $\mathbf{H} \in \Sigma_{[\mathbb{D}_2]}$ if $\mathbf{d}_2 \times \mathbf{d}_2^2 \neq 0$ or $\mathbf{c}_3 \times \mathbf{c}_3^2 \neq 0$ or $\mathbf{d}_2 \times \mathbf{c}_3 \neq 0$. Now, if $\mathbf{d}_2 \times \mathbf{d}_2^2 = 0$, $\mathbf{c}_3 \times \mathbf{c}_3^2 = 0$ and $\mathbf{d}_2 \times \mathbf{c}_3 = 0$ then $(\mathbf{d}_2, \mathbf{c}_3)$ is transversely isotropic ([91, theorem 8.5]) and hence $\mathbf{H} \in \Sigma_{[\mathbb{D}_4]}$ or $\mathbf{H} \in \Sigma_{[\mathbb{D}_3]}$ or $\mathbf{H} \in \Sigma_{[\mathrm{O}(2)]}$ ([91, theorem 9.4]). But the equation $3J_4 - J_2^2 = 0$ prevents $\mathbf{H}$ from being trigonal ([2, proposition 4.7]) so that in all cases we have $\mathbf{H} \in \overline{\Sigma}_{[\mathbb{D}_2]}$.

□

3.3 Reducible representations

3.3.1 Isotropy classes for a direct sum of irreducible representations

After considering the problem of finding the isotropy classes for irreducible representations, many were interested in solving the problem for a direct sum of irreducible representations. In particular, they have established the isotropy classes for SO(3) and O(3) tensorial representations (used to model constitutive laws in mechanics), based on the fact that every finite dimensional representation of a compact Lie group can be decomposed into a direct sum of irreducible representations, as mentioned in theorem 3.2.5. For instance, in 1996, Forte and Vianello [37] solved definitively the problem for the SO(3)-representation on the space of *elasticity tensors* (a set of fourth-order tensors). In that case, eight isotropy classes were found. Based on this method, the problem was solved for other constitutive laws. For example, 16 isotropy classes were obtained for the O(3)-representation on the space of *Piezoelectricity tensors* (a set of third-order tensors) [84, 113, 111, 82, 114]. Similar results were obtained for other constitutive tensor spaces [38, 66].

However, the Forte-Vianello approach requires rather fine calculations and reasoning to establish the classification. This complexity makes difficult its application to more involved situations, such as constitutive tensors of order greater than 4 or coupled constitutive laws involving a family of tensors [54, 33]. A systematic way to calculate the isotropy classes was proposed by Chossat and Guyard in [18] using a binary operation between conjugacy classes. This operation was named the *clips operation* in [87, 88, 86, 89], where it was generalized and used to determine isotropy classes for reducible representations.

3.3.2 Clips operation

Chossat and Guyard [18] found the isotropy classes of a direct sum of two irreducible SO(3)-representations. To do so, they introduced a binary operation on the conjugacy classes of closed SO(3)-subgroups that allows one to compute the set of isotropy classes $\mathcal{J}(V)$ of a direct sum $V = V_1 \oplus V_2$ of linear representations of a group G, if we know the isotropy classes for each individual representation. Such an operation has been generalized by Marc Olive [86] to all conjugacy classes of closed subgroups of a given group G and is defined as follows

Definition 3.3.1. *For two subgroups H_1 and H_2 of a group G, we define the* clips operation *of the conjugacy classes $[H_1]$ and $[H_2]$ as the set of conjugacy classes*

$$[H_1] \circledcirc [H_2] := \left\{ [H_1 \cap gH_2g^{-1}], \quad g \in G \right\}.$$

This definition extends to two families (finite or infinite) $\mathcal{F}_1$ and $\mathcal{F}_2$ of conjugacy classes

$$\mathcal{F}_1 \circledcirc \mathcal{F}_2 = \bigcup_{\substack{[H_i]\in\mathcal{F}_i \\ i\in\{1,2\}}} [H_1] \circledcirc [H_2].$$

The following lemma states a central result that is useful to find the isotropy classes of a reducible representation once we know the isotropy classes of irreducible ones (see [86, lemma 2.3] for a proof).

Lemma 3.3.2. *Let V_1 and V_2 be two linear representations of G. Then the set $\mathcal{J}(V_1 \oplus V_2)$ of isotropy classes of the representation of G on $V_1 \oplus V_2$ is given by*

$$\mathcal{J}(V_1 \oplus V_2) = \mathcal{J}(V_1) \circledcirc \mathcal{J}(V_2).$$

Using this result, one can find the isotropy classes of any representation V provided we know

1. a stable decomposition $V = W_1 \oplus \cdots \oplus W_r$,
2. the isotropy classes of each representations W_k, $k \in \{1, \ldots, r\}$,
3. the clips table of $[H_1] \circledcirc [H_2]$ for all conjugacy classes $[H_1], [H_2]$ of closed subgroups of G.

3.4 Clips operations between closed O(3)-subgroups

As recalled in section 3.1 (see also [53] for details), any closed O(3)-subgroup is either of type I, type II or type III. The clips tables have already been established for two type I subgroups

(see [18, table 1],[86, Table 1] and subsection 3.4.1) and for two type III subgroups (see [86, Table 2]). The clips operation between a type I and a type III subgroup is deduced from [86, Lemma 5.4]. The clips between a type I and a type II subgroup or two type II subgroups are deduced from the clips between two type I subgroups, see remark 3.4.1 below. However, the clips between type II and type III subgroups do not seem to have already been calculated. The main result of this chapter is their calculation, the results are summarized in tables 3.2 and 3.3 of the next section.

Remark 3.4.1. *Notice that*

1. *if H_1 and H_2 are two closed subgroups of* $\mathrm{SO}(3)$*, then,*

$$[H_1] \circledcirc [H_2 \oplus \mathbb{Z}_2^c] = [H_1] \circledcirc [H_2] \text{ and } [H_1 \oplus \mathbb{Z}_2^c] \circledcirc [H_2 \oplus \mathbb{Z}_2^c] = ([H_1] \circledcirc [H_2]) \oplus \mathbb{Z}_2^c.$$

2. *for every subgroup H of* $\mathrm{SO}(3)$ *we have*

$$[H] \circledcirc [\mathrm{O}(3)] = \{[H]\} \text{ and } [\mathbb{1}] \circledcirc [H] = \{[\mathbb{1}]\}.$$

3.4.1 Clips operations between closed $\mathrm{O}(3)$-subgroups of type I

The clips tables for SO(3)-subgroups can be found in [18, table 1] and [86, Table 1]. However, these two tables differ in some cases. In the following remark, we point out the differences between the two references and we recalculate the disputed clips.

Remark 3.4.2. *The two tables regrouping the clips between* $\mathrm{SO}(3)$*-subgroups provided in [18, table 1] and [86, Table 1] differ in the following cases:*

- *Clips between $[\mathbb{D}_n]$ and $[\mathrm{O}(2)]$ (see equations (3.10) and (3.16) for details on these subgroups): the table given by Chossat [18] is the correct one in this case*

$$[\mathbb{D}_n] \circledcirc [\mathrm{O}(2)] = \{[\mathbb{1}], [\mathbb{D}_n], [\mathbb{D}_2](\text{if } n \text{ is even}), [\mathbb{Z}_2]\}$$

  since Olive in [86] has $[\mathbb{D}_2]$ if n is odd instead of n even. Indeed, the following intersection

$$\mathbb{D}_n \cap g\mathrm{O}(2)g^{-1} = \left\{\mathbf{r}\left(\boldsymbol{e}_3, \frac{2k\pi}{n}\right), \mathbf{r}(\mathbf{b}_i, \pi)\right\} \cap \{\mathbf{r}(g\boldsymbol{e}_3, \theta), \mathbf{r}(g\mathbf{b}, \pi)\}$$

  gives $\mathbb{D}_2$ only if n is even (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$: $g\boldsymbol{e}_3 = -\boldsymbol{e}_1 = \mathbf{b}_1$ and $g\mathbf{b}_1 = -\boldsymbol{e}_3$).

- *Clips between $[\mathbb{T}]$ and $[\mathbb{T}]$: the table of Olive [86, table 1] is the correct one for this case*

$$[\mathbb{T}] \circledcirc [\mathbb{T}] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{Z}_3], [\mathbb{T}]\}$$

  since Chossat [18, table 1] omits the conjugacy class $[\mathbb{D}_2]$. Indeed, $[\mathbb{D}_2] \in [\mathbb{T}] \circledcirc [\mathbb{T}]$ since the intersection

$$\mathbb{T} \cap g\mathbb{T}g^{-1}, \quad \text{for } \mathbb{T} = \bigcup_{i=1}^{3} \mathbb{Z}_2^{\boldsymbol{e}_i} \cup \bigcup_{j=1}^{4} \mathbb{Z}_3^{\boldsymbol{s}_{t_j}} (3.11),$$

  gives $\mathbb{D}_2$ for $g = \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ for example.

- *Clips between* $[\mathbb{T}]$ *and* $[\mathbb{O}]$*: we follow the table given by Olive [86] for this case*

$$[\mathbb{T}] \circledcirc [\mathbb{O}] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{Z}_3], [\mathbb{T}]\}$$

since Chossat [18] omits the conjugacy class $[\mathbb{Z}_3]$*. Indeed,* $[\mathbb{Z}_3] \in [\mathbb{T}] \circledcirc [\mathbb{O}]$ *since the intersection*

$$\mathbb{O} \cap g\mathbb{T}g^{-1}, \quad \textit{for } \mathbb{T} = \bigcup_{i=1}^{3} \mathbb{Z}_2^{\boldsymbol{e}_i} \cup \bigcup_{j=1}^{4} \mathbb{Z}_3^{\boldsymbol{s}_{t_j}} (3.11), \textit{ and } \mathbb{O} = \bigcup_{i=1}^{3} \mathbb{Z}_4^{\boldsymbol{e}_i} \cup \bigcup_{j=1}^{4} \mathbb{Z}_3^{\boldsymbol{s}_{t_j}} \cup \bigcup_{k=1}^{6} \mathbb{Z}_2^{\boldsymbol{a}_{c_k}} (3.12),$$

gives $\mathbb{Z}_3$ *for* $g = \mathbf{r}\left(\boldsymbol{e}_2 - \boldsymbol{e}_3, \arccos(-\frac{1}{3})\right)$ *for example.*

- *Clips between* $[\mathbb{O}]$ *and* $[\mathbb{I}]$*: we consider the table 1 of Olive [86]*

$$[\mathbb{O}] \circledcirc [\mathbb{I}] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{D}_3], [\mathbb{T}]\}$$

since $[\mathbb{D}_2] \notin [\mathbb{O}] \circledcirc [\mathbb{I}]$*; the intersection*

$$\mathbb{O} \cap g\mathbb{I}g^{-1}, \quad \textit{for } \mathbb{I} = \bigcup_{i=1}^{6} \mathbb{Z}_5^{\boldsymbol{u}_i} \cup \bigcup_{j=1}^{10} \mathbb{Z}_3^{\boldsymbol{v}_j} \cup \bigcup_{k=1}^{15} \mathbb{Z}_2^{\boldsymbol{w}_k} (3.14),$$

gives $\mathbb{D}_2$ *only if there exists three orthogonal vectors* $\boldsymbol{w}_k$*,* $k = 1, \ldots, 15$*, that turn to* $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ *for some rotation* g*. However, the only three orthogonal vectors* $\boldsymbol{w}_k$ *which match this condition are the vectrs of the triplet* $(\boldsymbol{w}_4, \boldsymbol{w}_{10}, \boldsymbol{w}_{12})$*, and in that case the intersection gives* $\mathbb{T}$ *(since* g *is necessarily the identity rotation in that case).*

- *Clips between* $[\mathbb{I}]$ *and* $[\mathbb{I}]$*: the table given by Olive [86] is the correct one in this case*

$$[\mathbb{I}] \circledcirc [\mathbb{I}] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{D}_3], [\mathbb{Z}_5], [\mathbb{D}_5], [\mathbb{I}]\}$$

since Chossat has the conjugacy class $[\mathbb{T}]$ *which cannot be realized by any rotation using the intersection* $\mathbb{I} \cap g\mathbb{I}g^{-1}$ *(the only rotation that could realize* $\mathbb{T}$ *is the identity rotation which gives* $\mathbb{I}$ *instead).*

3.4.2 Clips operations between type II and type III subgroups: results

We give, in tables 3.2 and 3.3, clips operations between type II and type III subgroups, where we have used the notations

$$d := \gcd(m, n), \quad d_k := \gcd(k, n), \quad d'_k := \gcd(k, m),$$

$$\mathcal{Z}(n) := \begin{cases} [\mathbb{Z}_2] & \text{if } n \text{ even} \\ [\mathbb{Z}_2^-] & \text{else} \end{cases} \text{ and } \mathsf{L}_{\mathbb{O}} := [\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_{d_2}], [\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{Z}_{d_3}], [\mathbb{D}_{d_3}], [\mathbb{D}_{d_3}^z].$$

Remark 3.4.3. *In the following tables we have used the conventions*

$$[\mathbb{Z}_1] := [\mathbb{1}], \quad [\mathbb{D}_1] = [\mathbb{Z}_2], \quad [\mathbb{D}_1^z] = [\mathbb{Z}_2^-], \quad [\mathbb{D}_2^z] = [\mathbb{D}_2^d].$$

$\circledcirc$	$[\mathbb{Z}_{2n}^-]$	$[\mathbb{D}_n^z]$	$[\mathbb{D}_{2n}^d]$
$[\mathbb{Z}_m \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_{2d}^-]$ if $\frac{m}{d}$ even $[\mathbb{1}], [\mathbb{Z}_d]$ else	$[\mathbb{1}], [\mathbb{Z}_d]$ if m odd $[\mathbb{1}], [\mathbb{Z}_d], [\mathbb{Z}_2^-]$ else	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_{2d}^-]$ if $\frac{m}{d}$ even $[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_d]$ if m even and $\frac{m}{d}$ odd $[\mathbb{1}], [\mathbb{Z}_d]$ else
$[\mathbb{D}_m \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_{2d}^-], \mathcal{Z}(n)$ if $\frac{m}{d}$ even $[\mathbb{1}], [\mathbb{Z}_d], \mathcal{Z}(n)$ else	$[\mathbb{1}], [\mathbb{Z}_d], [\mathbb{Z}_{d_2}]$ $[\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z], [\mathbb{D}_d^z]$ if m even $[\mathbb{1}], [\mathbb{Z}_d]$ $[\mathbb{Z}_{d_2}], [\mathbb{Z}_2^-], [\mathbb{D}_d^z]$ else	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_{d_2}], [\mathbb{Z}_2^-]$ $[\mathbb{Z}_{2d}^-], [\mathbb{D}_2^z], [\mathbb{D}_{2d}^d]$ if $\frac{m}{d}$ even $[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{Z}_2^-]$ $[\mathbb{D}_2^z], [\mathbb{Z}_d], [\mathbb{D}_d], [\mathbb{D}_d^z]$ if m even and $\frac{m}{d}$ odd $[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_d], [\mathbb{D}_d], [\mathbb{D}_d^z]$ else
$[\mathbb{O} \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_2]$ $[\mathbb{Z}_{d_3}], [\mathbb{Z}_4]$ if $4\|n$ $[\mathbb{1}], [\mathbb{Z}_2]$ $[\mathbb{Z}_{d_3}], [\mathbb{Z}_4^-]$ if n even and $4 \nmid n$ $[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{Z}_{d_3}]$ else	$[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_4}]$ $[\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z], [\mathbb{D}_{d_3}^z], [\mathbb{D}_{d_4}^z]$	$\mathsf{L}_{\mathbb{O}}, [\mathbb{Z}_4^-]$ $[\mathbb{Z}_4], [\mathbb{D}_4], [\mathbb{D}_4^z]$ if $4\|n$ $\mathsf{L}_{\mathbb{O}}, [\mathbb{Z}_4^-], [\mathbb{D}_4^d]$ if n even and $4 \nmid n$ $\mathsf{L}_{\mathbb{O}}$ else
$[\mathbb{T} \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_{d_3}], \mathcal{Z}(n)$	$[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}], [\mathbb{D}_{d_2}^z]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}], [\mathbb{D}_2^z], [\mathbb{Z}_{d_3}]$
$[\mathbb{I} \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], \mathcal{Z}(n), [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_5}]$	$[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}]$ $[\mathbb{Z}_{d_5}], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}], [\mathbb{D}_2^z], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_5}]$
$[\mathrm{SO}(2) \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_{2n}^-]$	$[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{Z}_n]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_{2n}^-]$
$[\mathrm{O}(2) \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], \mathcal{Z}(n), [\mathbb{Z}_{2n}^-]$	$[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z], [\mathbb{D}_n^z]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}], [\mathbb{D}_2^z], [\mathbb{D}_{2n}^d]$

Table 3.2: Clips between type II and III O(3)-subgroups (part 1)

$\circledcirc$	$[\mathbb{O}^-]$	$[\mathrm{O}(2)^-]$
$[\mathbb{Z}_m \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_{d'_3}], [\mathbb{Z}_2^-], [\mathbb{Z}_4^-]$ if $4\|m$ $[\mathbb{1}], [\mathbb{Z}_{d'_2}], [\mathbb{Z}_{d'_3}], [\mathbb{Z}_{d'_2}^-]$ else	$[\mathbb{1}], [\mathbb{Z}_m], [\mathbb{Z}_{d'_2}^-]$
$[\mathbb{D}_m \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d'_3}], [\mathbb{Z}_2^-]$ $[\mathbb{Z}_4^-], [\mathbb{D}_{d'_3}^z], [\mathbb{D}_2^z], [\mathbb{D}_4^d]$ if $4\|m$ $[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d'_3}], [\mathbb{Z}_2^-]$ $[\mathbb{D}_2], [\mathbb{D}_{d'_3}^z], [\mathbb{D}_2^z]$ if m even and $4 \nmid m$ $[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d'_3}], [\mathbb{Z}_2^-], [\mathbb{D}_{d'_3}^z]$ else	$[\mathbb{1}], [\mathbb{Z}_2^-]$ $[\mathbb{D}_2^z], [\mathbb{D}_m^z]$ if m even $[\mathbb{1}], [\mathbb{Z}_2]$ $[\mathbb{Z}_2^-], [\mathbb{D}_m^z]$ else
$[\mathbb{O} \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{Z}_2^-], [\mathbb{Z}_4^-], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{D}_4^d], [\mathbb{O}^-]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{D}_4^z]$
$[\mathbb{T} \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{Z}_2^-], [\mathbb{D}_2], [\mathbb{D}_2^z], [\mathbb{T}]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{Z}_2^-], [\mathbb{D}_2^z]$
$[\mathbb{I} \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_2], [\mathbb{D}_2^z], [\mathbb{Z}_3], [\mathbb{T}]$	$[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_2^z]$
$[\mathrm{SO}(2) \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_3], [\mathbb{Z}_2^-], [\mathbb{Z}_4^-]$	$[\mathbb{1}], [\mathbb{Z}_2^-], [\mathrm{SO}(2)]$
$[\mathrm{O}(2) \oplus \mathbb{Z}_2^c]$	$[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{D}_3^z], [\mathbb{D}_4^d]$	$[\mathbb{D}_2^z], [\mathrm{O}(2)^-]$

Table 3.3: Clips between type II and III O(3)-subgroups (part 2)

3.5 Clips operations between type II and type III O(3)-subgroups: calculations

Let $\Gamma = \Gamma_+ \cup (-\gamma\Gamma_+)$ $(-\gamma \in \Gamma \setminus \Gamma_+)$ be a subgroup of type III (see section 3.1) and H a subgroup of SO(3). By definition, the clips operation between a type II and a type III subgroups $[\Gamma] \circledcirc [H \oplus \mathbb{Z}_2^c]$ is given by the intersection $\Gamma \cap (gHg^{-1} \oplus \mathbb{Z}_2^c)$ which can be reduced to

$$\Gamma \cap (gHg^{-1} \oplus \mathbb{Z}_2^c) = (\Gamma_+ \cap (gHg^{-1})) \cup (-(\gamma\Gamma_+ \cap (gHg^{-1}))), \quad -\gamma \in \Gamma \setminus \Gamma_+ \tag{3.18}$$

Indeed, as we have $H \oplus \mathbb{Z}_2^c = H \cup (-H)$ we deduce that

$$\begin{aligned}\Gamma \cap (H \oplus \mathbb{Z}_2^c) &= (\Gamma_+ \cup (-\gamma\Gamma_+)) \cap (H \cup (-H)) \\ &= (\Gamma_+ \cap H) \cup (\Gamma_+ \cap (-H)) \cup (-(\gamma\Gamma_+) \cap H) \cup (-(\gamma\Gamma_+) \cap (-H)) \\ &= (\Gamma_+ \cap H) \cup (-((\gamma\Gamma_+) \cap H)).\end{aligned}$$

In the following, we prove a theorem which describes the possible conjugacy classes belonging to the clips between a type II and type III subgroups of O(3). The computation of such classes can be complicated since it involves intersection of groups of type III which can be tricky sometimes

and we would risk to not cover all the groups resulting from this intersection. For this reason, we use a characterization of these conjugacy classes making use of the clips between type I subgroups that have already been calculated before (see subsection 3.4.1). But, before this, a preparatory lemma is needed.

Lemma 3.5.1. *Let $(K_+, \tilde{K})$ be a pair of subgroups of a group G of index 2 and H be a subgroup of G. Then, either*

$$K_+ \cap H = \tilde{K} \cap H, \text{ or the pair } (K_+ \cap H, \tilde{K} \cap H) \text{ is of index 2.}$$

Proof. Consider the following exact sequence

$$\mathbb{1} \to K_+ \xrightarrow{i} \tilde{K} \xrightarrow{p} \tilde{K}/K_+ \simeq \mathbb{Z}_2 \to \mathbb{1}$$

Then $p(\tilde{K} \cap H)$ is a subgroup of $\mathbb{Z}_2$. Therefore, either $p(\tilde{K} \cap H) = \mathbb{Z}_2$ and in this case $(K_+ \cap H, \tilde{K} \cap H)$ is a pair of index 2 (considering the exact sequence $\mathbb{1} \to K_+ \cap H \to \tilde{K} \cap H \to \mathbb{Z}_2$) or $p(\tilde{K} \cap H) = \mathbb{1}$ and then $\tilde{K} \cap H = K_+ \cap H$. □

Theorem 3.5.2. *Let Γ be a type III subgroup of $\mathrm{O}(3)$, built from a pair of $\mathrm{SO}(3)$-subgroups $(\Gamma_+, \tilde{\Gamma})$ of index 2 and let H be a subgroup of $\mathrm{SO}(3)$. Let L be a subgroup of $\mathrm{O}(3)$ such that $[L] \in [\Gamma] \circledcirc [H \oplus \mathbb{Z}_2^c]$ then, either*

1. *L is of type I and $[L] \in ([\Gamma_+] \circledcirc [H]) \cap ([\tilde{\Gamma}] \circledcirc [H])$,*
2. *or L is of type III built from a pair $(L_+, \tilde{L})$ of index 2 such that $[L_+] \in [\Gamma_+] \circledcirc [H]$ and $[\tilde{L}] \in [\tilde{\Gamma}] \circledcirc [H]$.*

Proof. First, remark that $-\mathrm{I}$ does not belong to the intersection between a type II and a type III subgroups and hence if $[L] \in [\Gamma] \circledcirc [H \oplus \mathbb{Z}_2^c]$ then L is either of type I or type III. Let $[L] \in [\Gamma] \circledcirc [H \oplus \mathbb{Z}_2^c]$ then $[L]$ is given by the union (3.18)

$$L = \Gamma_+ \cap gHg^{-1} \cup (-(\gamma\Gamma_+ \cap gHg^{-1})), \quad g \in \mathrm{SO}(3),\ \gamma \in \tilde{\Gamma} \setminus \Gamma_+.$$

If $\gamma\Gamma_+ \cap gHg^{-1} = \emptyset$ then L is of type I and $L = \Gamma_+ \cap gHg^{-1} = \tilde{\Gamma} \cap gHg^{-1}$. Hence, $[L] \in ([\Gamma_+] \circledcirc [H]) \cap ([\tilde{\Gamma}] \circledcirc [H])$.

If $\gamma\Gamma_+ \cap gHg^{-1} \neq \emptyset$ then L is of type III and $\Gamma_+ \cap gHg^{-1} \neq \tilde{\Gamma} \cap gHg^{-1}$. Since $(\Gamma_+, \tilde{\Gamma})$ is a pair of index 2 then, by lemma 3.5.1, the pair $(\Gamma_+ \cap gHg^{-1}, \tilde{\Gamma} \cap gHg^{-1})$ is of index 2. Hence, there exists $\sigma \in \tilde{\Gamma} \cap gHg^{-1} \setminus (\Gamma_+ \cap gHg^{-1})$ such that

$$L = \Gamma_+ \cap gHg^{-1} \cup (-\sigma(\Gamma_+ \cap gHg^{-1}))$$

Hence the result. □

In the next subsections, we compute the clips operation between type II and type III subgroups of $\mathrm{O}(3)$ using theorem 3.5.2 which involves clips between type I $\mathrm{O}(3)$-subgroups that have already been calculated in previous works ([18, 86], see also remark 3.4.2). Indeed, the classes for the clips operation between a subgroup $H \oplus \mathbb{Z}_2^c$ of type II and a subgroup Γ of type III are

deduced from the knowledge of the tables of the clips $[\Gamma_+] \circledcirc [H]$ and $[\tilde{\Gamma}] \circledcirc [H]$. By eliminating the classes that cannot be realized by any $g \in \mathrm{SO}(3)$, we deduce the clips operation between $[\Gamma]$ and $[H \oplus \mathbb{Z}_2^c]$.

3.5.1 Clips with $\mathbb{Z}_{2n}^-$

First, let us recall that $\mathbb{Z}_{2n}^-$ is built from the couple $(\mathbb{Z}_n, \mathbb{Z}_{2n})$, where $\mathbb{Z}_n$ is given by (3.9), as in the equation (3.3) of section 3.1

$$\mathbb{Z}_{2n}^- = \mathbb{Z}_n \cup (-\gamma \mathbb{Z}_n), \quad \gamma = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{n}\right)$$

where we denote $\mathbb{Z}_1 := \{\mathrm{I}\}$ when $n = 1$.

Lemma 3.5.3. *Let $n \geq 1$ and $m \geq 2$ be two integers and $d = \gcd(m, n)$. Then*

$$[\mathbb{Z}_{2n}^-] \circledcirc [\mathbb{Z}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_{2d}^-]\} & \text{if } \frac{m}{d} \text{ even}, \\ \{[\mathbb{1}], [\mathbb{Z}_d]\} & \text{else}. \end{cases}$$

Proof. We deduce from (3.18) that

$$\mathbb{Z}_{2n}^- \cap (g\mathbb{Z}_m g^{-1} \oplus \mathbb{Z}_2^c) = (\mathbb{Z}_n \cap g\mathbb{Z}_m g^{-1}) \cup (-(\gamma \mathbb{Z}_n \cap g\mathbb{Z}_m g^{-1})), \quad \gamma = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{n}\right).$$

In the case when $g\boldsymbol{e}_3$ and $\boldsymbol{e}_3$ are not colinear, such group reduces to $\mathbb{1}$, so we suppose now that $g\boldsymbol{e}_3 = \pm\boldsymbol{e}_3$. We thus have to consider

$$(\mathbb{Z}_n \cap \mathbb{Z}_m) \cup (-(\gamma \mathbb{Z}_n \cap \mathbb{Z}_m))$$

where $\mathbb{Z}_n \cap \mathbb{Z}_m = \mathbb{Z}_d$, and $\gamma \mathbb{Z}_n \cap \mathbb{Z}_m$ is obtained by solving the equations of unknown $k_1, k_2 \in \mathbb{Z}$

$$\frac{2k_1 + 1}{n} = \frac{2k_2}{m}. \tag{3.19}$$

If $m = m_1 d$ and $n = n_1 d$, for $m_1, n_1 \in \mathbb{N}$, then the equation (3.19) becomes $(2k_1 + 1)dm_1 = 2k_2 dn_1$ with $\gcd(m_1, n_1) = 1$. We get solutions only if $m_1 = \frac{m}{d}$ is even. By replacing m_1 by $2p$ we get that p divides k_2 hence $k_2 = pk'$. Replacing m_1 by $2p$ and k_2 by pk' in the equation $(2k_1 + 1)dm_1 = 2k_2 dn_1$ we get that k' is odd. On one hand, $\frac{2k_2}{m} = \frac{2pk'}{2pd}$ and on the other hand, $\frac{2k_1+1}{n} = \frac{k'n_1}{dn_1}$ with k' odd. If we write $k' = 2k + 1$ such that $k \in \mathbb{N}$, then

$$\gamma \mathbb{Z}_n \cap \mathbb{Z}_m = \left\{\mathbf{r}\left(\boldsymbol{e}_3, \frac{(2k+1)\pi}{d}\right)\right\}.$$

□

In the following, recall that

$$\mathcal{Z}(n) := \mathbb{Z}_{2n}^- \circledcirc (\mathbb{Z}_2 \oplus \mathbb{Z}_2^c) = \begin{cases} [\mathbb{Z}_2] & \text{if } n \text{ even}, \\ [\mathbb{Z}_2^-] & \text{else}. \end{cases} \tag{3.20}$$

Lemma 3.5.4. *Let $n \geq 1$ and $m \geq 2$ be two integers and $d = \gcd(m,n)$. Then*

$$[\mathbb{Z}_{2n}^-] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_{2d}^-], \mathcal{Z}(n)\} & \text{if } \frac{m}{d} \text{ even,} \\ \{[\mathbb{1}], [\mathbb{Z}_d], \mathcal{Z}(n)\} & \text{else.} \end{cases}$$

Proof. Recall from (3.10) that

$$\mathbb{D}_m = \mathbb{Z}_m \cup_{i=1}^m \mathbb{Z}_2^{\mathbf{b}_i}, \quad \mathbb{Z}_2^{\mathbf{b}_i} := \{e, \mathbf{r}(\mathbf{b}_i, \pi)\}$$

where $\mathbf{b}_i$ are called the secondary axes of the subgroup $\mathbb{D}_m$, with

$$\mathbf{b}_1 = \boldsymbol{e}_1, \quad \mathbf{b}_k = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{m}\right)\mathbf{b}_{k-1}, \quad k = 2, \ldots, m.$$

We have

$$\mathbb{Z}_{2n}^- \cap (g\mathbb{D}_m g^{-1} \oplus \mathbb{Z}_2^c) = \left(\mathbb{Z}_n \cap g\mathbb{D}_m g^{-1}\right) \bigcup \left(-(\gamma\mathbb{Z}_n \cap (g\mathbb{D}_m g^{-1}))\right).$$

The non-trivial cases take place for $g\boldsymbol{e}_3 = \pm\boldsymbol{e}_3$ and the union is then deduced from lemma 3.5.3, and for $g\mathbf{b}_i = \pm\boldsymbol{e}_3$ in which case we get $\mathcal{Z}(n)$, hence the conclusion. □

Lemma 3.5.5. *Let $n \geq 1$, $d_3 = \gcd(3,n)$ and $d_5 = \gcd(5,n)$. We have*

$$[\mathbb{Z}_{2n}^-] \circledcirc [\mathbb{T} \oplus \mathbb{Z}_2^c] = \{[\mathbb{1}], [\mathbb{Z}_{d_3}], \mathcal{Z}(n)\}, \quad [\mathbb{Z}_{2n}^-] \circledcirc [\mathbb{I} \oplus \mathbb{Z}_2^c] = \{[\mathbb{1}], \mathcal{Z}(n), [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_5}]\}.$$

$$[\mathbb{Z}_{2n}^-] \circledcirc [\mathbb{O} \oplus \mathbb{Z}_2^c] = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3}], [\mathbb{Z}_4]\} & \text{if } n \text{ is even and } 4|n, \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3}], [\mathbb{Z}_4^-]\} & \text{if } n \text{ is even but } 4 \nmid n, \\ \{[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{Z}_{d_3}]\} & \text{if } n \text{ is odd.} \end{cases}$$

Proof. By (3.18), we have to consider

$$(\mathbb{Z}_n \cap (gHg^{-1})) \cup (-(\gamma\mathbb{Z}_n \cap (gHg^{-1}))) \text{ for } H = \mathbb{T}, \mathbb{O}, \mathbb{I}.$$

Let us consider decomposition (3.11) of the group $\mathbb{T}$. Then the only non-trivial cases are obtained for $g\boldsymbol{e}_i = \pm\boldsymbol{e}_3$ in which case we get $\mathcal{Z}(n)$, and for $g\mathbf{s}_{t_j} = \pm\boldsymbol{e}_3$ we get $\mathbb{Z}_{d_3}$.

For the group $\mathbb{O}$ given in (3.12), the only non-trivial cases are for $g\mathbf{a}_{c_k} = \pm\boldsymbol{e}_3$ and $g\mathbf{s}_{t_j} = \pm\boldsymbol{e}_3$ which have been calculated in the case of $\mathbb{T}$, and for $g\boldsymbol{e}_i = \pm\boldsymbol{e}_3$ in which case we get $\mathbb{Z}_4$ if $4 \mid n$, $\mathbb{Z}_4^-$ if n is even but $4 \nmid n$ and $\mathbb{Z}_2^-$ otherwise.

For the group $\mathbb{I}$, we consider the decomposition (3.14) and we deduce the result following the same reasoning. □

Finally, for the subgroups SO(2) and O(2) given in (3.15) and (3.16) and as a direct consequence of (3.18),

Lemma 3.5.6. *For any integer $n \geq 1$ we have:*

$$[\mathbb{Z}_{2n}^-] \circledcirc [\mathrm{SO}(2) \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_{2n}^-]\right\}, \quad [\mathbb{Z}_{2n}^-] \circledcirc [\mathrm{O}(2) \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], \mathcal{Z}(n), [\mathbb{Z}_{2n}^-]\right\}$$

with $\mathcal{Z}(n)$ given by (3.20).

3.5.2 Clips with $\mathbb{D}_n^z$

As explained in section 3.1, the subgroup $\mathbb{D}_n^z$ is obtained for $-\gamma = -\mathbf{r}(\mathbf{e}_1, \pi)$, so that

$$\mathbb{D}_n^z = \mathbb{Z}_n \cup -\gamma\mathbb{Z}_n = \mathbb{Z}_n \cup \{-\mathbf{r}(\mathbf{b}_1, \pi), \ldots, \ -\mathbf{r}(\mathbf{b}_n, \pi)\}, \quad \mathbf{b}_1 = \boldsymbol{e}_1, \quad \mathbf{b}_k = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{n}\right)\mathbf{b}_{k-1}, \ k = 2, \ldots, n$$

where $\mathbf{b}_i$, $i \in \{1, \ldots, n\}$, are called secondary axes of the dihedral subgroup $\mathbb{D}_n$ (see [86, Appendix A]).

Lemma 3.5.7. *Let $m, \ n \geq 2$ be two integers and $d = \gcd(m, n)$. Then*

$$[\mathbb{D}_n^z] \circledcirc [\mathbb{Z}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_d]\} & \textit{if } m \textit{ is odd,} \\ \{[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{Z}_d]\} & \textit{if } m \textit{ is even.} \end{cases}$$

Proof. From (3.18) we have to consider

$$\mathbb{D}_n^z \cap (g\mathbb{Z}_m g^{-1} \oplus \mathbb{Z}_2^c) = (\mathbb{Z}_n \cap g\mathbb{Z}_m g^{-1}) \cup (-(\gamma\mathbb{Z}_n \cap g\mathbb{Z}_m g^{-1})), \quad \gamma = \mathbf{r}(\mathbf{e}_1, \pi),$$

where $\gamma\mathbb{Z}_n = \{\mathbf{r}(\mathbf{b}_1, \pi), \ldots, \ \mathbf{r}(\mathbf{b}_n, \pi)\}$. Here, the only non–trivial cases are obtained when $g\mathbb{Z}_m g^{-1} = \mathbb{Z}_n$ (see lemma 3.5.3) or $\mathbb{Z}_2^{\mathbf{b}_i}$, which leads directly to the result. □

Lemma 3.5.8. *Let $m, \ n \geq 2$ be two integers and $d = \gcd(m, n)$ and $d_2 = \gcd(2, n)$. Then*

$$[\mathbb{D}_n^z] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \left\{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_d], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z], [\mathbb{D}_d^z]\right\} & \textit{if } m \textit{ is even,} \\ \left\{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_d], [\mathbb{Z}_2^-], [\mathbb{D}_d^z]\right\} & \textit{if } m \textit{ is odd.} \end{cases}$$

Proof. We apply theorem 3.5.2 with $\Gamma_+ = \mathbb{Z}_n$ and $\tilde{\Gamma} = \mathbb{D}_n$. We have from [86, table 1]

$$[\mathbb{Z}_n] \circledcirc [\mathbb{D}_m] = \{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_d]\} \text{ and } [\mathbb{D}_n] \circledcirc [\mathbb{D}_m] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2](\text{if } m \text{ and } n \text{ even}), [\mathbb{Z}_d], [\mathbb{D}_d]\}$$

Hence, the classes of $[\mathbb{D}_n^z] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\Gamma_+] \circledcirc [H]) \cap ([\tilde{\Gamma}] \circledcirc [H]) = \{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_d]\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z](\text{ if } m \text{ is even}), [\mathbb{D}_d^z]\right\}.$$

We can check that all the eventualities can occur by using (3.18):

$$(\mathbb{Z}_n \cap g\mathbb{D}_m g^{-1}) \cup (-(\gamma\mathbb{Z}_n \cap g\mathbb{D}_m g^{-1}))$$

where $\gamma\mathbb{Z}_n = \{\mathbf{r}(\mathbf{b}_i, \pi), i = 1, \ldots, n\}$ and $\mathbb{D}_m = \mathbb{Z}_m \cup_{j=1}^m \mathbb{Z}_2^{\mathbf{b}_j}$, we get

- $[\mathbb{Z}_{d_2}]$ for a rotation g such that, $\exists j = 1, \ldots, m$, $g\mathbf{b}_j = \boldsymbol{e}_3$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ that turns only $\boldsymbol{e}_1$ to $\boldsymbol{e}_3$ and nothing else),

- $[\mathbb{Z}_d]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{e}_3$ (for instance $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{3}\right)$),
- $[\mathbb{Z}_2^-]$ for a rotation g such that, $\exists j = 1, \ldots, m$ and $\exists i = 1, \ldots, n$, $g\mathbf{b}_j = \mathbf{b}_i$ (for instance $g = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{3}\right)$),
- $[\mathbb{D}_d^z]$ for the identity rotation for instance,
- $[\mathbb{D}_{d_2}^z]$ if m is even and in this case we can take $g = \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ for instance so that we have $g\boldsymbol{e}_3 = \boldsymbol{e}_1 = \mathbf{b}_1$ and $g\mathbf{b}_2 = \mathbf{b}_2 = \boldsymbol{e}_2$.

□

Lemma 3.5.9. *Let $n \geq 2$ be an integer, $d_2 = \gcd(2, n)$ and $d_3 = \gcd(3, n)$. We have*

$$[\mathbb{D}_n^z] \circledcirc [\mathbb{T} \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}], [\mathbb{D}_{d_2}^z]\right\}.$$

Proof. We deduce from [86, table 1] and theorem 3.5.2 that the classes in $[\mathbb{D}_n^z] \circledcirc [\mathbb{T} \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{Z}_n] \circledcirc [\mathbb{T}]) \cap ([\mathbb{D}_n] \circledcirc [\mathbb{T}]) = \{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}]\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z]\right\}.$$

We can check that all the eventualities can occur by using (3.18):

$$(\mathbb{Z}_n \cap g\mathbb{T}g^{-1}) \cup (-(\gamma\mathbb{Z}_n \cap g\mathbb{T}g^{-1}))$$

where $\gamma\mathbb{Z}_n = \{\mathbf{r}(\mathbf{b}_i, \pi), i = 1, \ldots, n\}$ and $\mathbb{T} = \bigcup_{i=1}^3 \mathbb{Z}_2^{\boldsymbol{e}_i} \bigcup_{j=1}^4 \mathbb{Z}_3^{\boldsymbol{s}_{t_j}}$ (3.11), we get

- $[\mathbb{Z}_2^-]$ for a rotation g such that $\exists i = 1, \ldots, n$, $g\boldsymbol{e}_1 = \mathbf{b}_i$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{3}\right)$),
- $[\mathbb{Z}_{d_2}]$ for a rotation g such that $\exists i = 1, \ldots, n$, $g\boldsymbol{e}_3 = \boldsymbol{e}_3$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{3}\right)$),
- $[\mathbb{Z}_{d_3}]$ for a rotation g such that $\exists j = 1, \ldots, 4$, $g\boldsymbol{s}_{t_j} = \boldsymbol{e}_3$,
- $[\mathbb{D}_{d_2}^z]$ for a rotation g such that $\exists i = 1, \ldots, 3$, $g\boldsymbol{e}_i = \boldsymbol{e}_3$ and the two remaining $\boldsymbol{e}_i$ turn to two orthogonal $\mathbf{b}_i$ (exists for n even).

□

Lemma 3.5.10. *Let $n \geq 2$ be an integer, $d_2 = \gcd(2, n)$, $d_3 = \gcd(3, n)$ and $d_4 = \gcd(4, n)$. We have*

$$[\mathbb{D}_n^z] \circledcirc [\mathbb{O} \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_4}], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z], [\mathbb{D}_{d_3}^z], [\mathbb{D}_{d_4}^z]\right\}.$$

Proof. We deduce from [86, table 1] and theorem 3.5.2 that the classes in $[\mathbb{D}_n^z] \circledcirc [\mathbb{O} \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{Z}_n] \circledcirc [\mathbb{O}]) \cap ([\mathbb{D}_n] \circledcirc [\mathbb{O}]) = \{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_4}]\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}_2^-], [\mathbb{D}{d_2}^z], [\mathbb{D}_{d_3}^z], [\mathbb{D}_{d_4}^z]\right\}.$$

We can check that all the eventualities can occur by using (3.18):

$$(\mathbb{Z}_n \cap g\mathbb{O}g^{-1}) \cup (-(\gamma\mathbb{Z}_n \cap g\mathbb{O}g^{-1}))$$

where $\mathbb{O} = \bigcup_{i=1}^{3} \mathbb{Z}_4^{\boldsymbol{e}_i} \bigcup_{j=1}^{4} \mathbb{Z}_3^{\boldsymbol{s}_{t_j}} \bigcup_{k=1}^{6} \mathbb{Z}_2^{\boldsymbol{a}_{c_k}}$ (3.12), we get

- $[\mathbb{Z}_2^-]$ for a rotation g such that, , $\exists k = 1, \ldots, 6$ and $\exists i = 1, \ldots, n$, $g\boldsymbol{a}_{c_k} = \mathbf{b}_i$ (for instance take $g = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, -\frac{\pi}{4}\right)$ that turns only $\boldsymbol{a}_{c_1}$ to $\boldsymbol{e}_1$),
- $[\mathbb{Z}_{d_2}]$ for a rotation g such that, $\exists k = 1, \ldots, 6$, $g\boldsymbol{a}_{c_k} = \boldsymbol{e}_3$,
- $[\mathbb{Z}_{d_3}]$ for a rotation g such that, $\exists j = 1, \ldots, 4$, $g\boldsymbol{s}_{t_j} = \boldsymbol{e}_3$,
- $[\mathbb{Z}_{d_4}]$ for a rotation g such that, $\exists i = 1, \ldots, 3$, $g\boldsymbol{e}_i = \boldsymbol{e}_3$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{2}\right)$),
- $[\mathbb{D}_{d_2}^z]$ for a rotation g such that, $\exists i = 1, \ldots, 6$, $g\boldsymbol{a}_{c_k} = \boldsymbol{e}_3$ and two other edge axes $\boldsymbol{a}_{c_k}$ turn to two orthogonal axes $\pm\mathbf{b}_i$ for $i = 1, \ldots, n$ (such g exists for n even),
- $[\mathbb{D}_{d_3}^z]$ for a rotation g such that $g\boldsymbol{s}_{t_j} = \boldsymbol{e}_3$ and three other edge axes $\boldsymbol{a}_{c_k}$ (for instance $\boldsymbol{a}_{c_1}, \boldsymbol{a}_{c_4}$ and $\boldsymbol{a}_{c_5}$ are three coplanar edge axes separated by an angle of $\frac{\pi}{3}$) turn to three $\pm\mathbf{b}_i$,
- $[\mathbb{D}_{d_4}^z]$ for $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{4}\right)$ for example.

□

Lemma 3.5.11. *Let $n \geq 2$ be an integer, $d_2 = \gcd(2, n)$, $d_3 = \gcd(3, n)$ and $d_5 = \gcd(5, n)$. We have*

$$[\mathbb{D}_n^z] \circledcirc [\mathbb{I} \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_5}], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z]\right\}.$$

Proof. We deduce from [86, table 1] and theorem 3.5.2 that the classes in $[\mathbb{D}_n^z] \circledcirc [\mathbb{I} \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{Z}_n] \circledcirc [\mathbb{I}]) \cap ([\mathbb{D}_n] \circledcirc [\mathbb{I}]) = \{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_5}]\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}_2^-], [\mathbb{D}_{d_2}^z], [\mathbb{D}_{d_3}^z], [\mathbb{D}_{d_5}^z]\right\}.$$

We can check that all the eventualities can occur, except $[\mathbb{D}_{d_3}^z]$ and $[\mathbb{D}_{d_5}^z]$, by using (3.18):

$$(\mathbb{Z}_n \cap g\mathbb{I}g^{-1}) \cup (-(\gamma\mathbb{Z}_n \cap g\mathbb{I}g^{-1}))$$

where $\mathbb{I} = \bigcup_{i=1}^{6} \mathbb{Z}_5^{\boldsymbol{u}_i} \bigcup_{j=1}^{10} \mathbb{Z}_3^{\boldsymbol{v}_j} \bigcup_{k=1}^{15} \mathbb{Z}_2^{\boldsymbol{w}_k}$ (3.14), we get

- $[\mathbb{Z}_2^-]$ for a rotation g such that, $\exists i = 1, \ldots, n$ and $\exists k = 1, \ldots, 15$, $g\boldsymbol{w}_k = \mathbf{b}_i$,

- $[\mathbb{Z}_{d_2}]$ for a rotation g such that, $\exists k = 1, \ldots, 15$, $g\boldsymbol{w}_k = \boldsymbol{e}_3$,
- $[\mathbb{Z}_{d_3}]$ for a rotation g such that, $\exists j = 1, \ldots, 10$, $g\boldsymbol{v}_j = \boldsymbol{e}_3$,
- $[\mathbb{Z}_{d_5}]$ for a rotation g such that, $\exists i = 1, \ldots, 6$, $g\boldsymbol{u}_i = \boldsymbol{e}_3$,
- $[\mathbb{D}^z_{d_2}]$ for a rotation g such that $g\boldsymbol{w}_k = \boldsymbol{e}_3$ and two other axes $\boldsymbol{w}_k$ turn to two orthogonal axes $\mathbf{b}_i$ for $i = 1, \ldots, n$ (such a g exists for n even) (the identity rotation works as well since $\boldsymbol{w}_4$, $\boldsymbol{w}_{10}$, $\boldsymbol{w}_{12}$ are colinear to $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ ($\boldsymbol{e}_2 = \mathbf{b}_i$ for some i for n even)),
- $[\mathbb{D}^z_{d_3}]$ for a rotation g such that $g\boldsymbol{v}_j = \boldsymbol{e}_3$ and three other axes $\boldsymbol{w}_j$ turn to three $\mathbf{b}_i$. However, there is no three coplanar $\boldsymbol{w}_k$ separated by an angle of $\frac{\pi}{3}$,
- $[\mathbb{D}^z_{d_5}]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{e}_3$ and five axes $\boldsymbol{w}_i$ turn to five $\mathbf{b}_i$. However, there is no five coplanar $\boldsymbol{w}_k$ separated by angle of $\frac{\pi}{5}$.

□

Lemma 3.5.12. *For any integer $n \geq 2$, we have*

$$[\mathbb{D}^z_n] \circledcirc [\mathrm{SO}(2) \oplus \mathbb{Z}^c_2] = \left\{[\mathbb{1}], [\mathbb{Z}^-_2], [\mathbb{Z}_n]\right\}$$
$$[\mathbb{D}^z_n] \circledcirc [\mathrm{O}(2) \oplus \mathbb{Z}^c_2] = \left\{[\mathbb{1}], [\mathbb{Z}^-_2], [\mathbb{D}^z_{d_2}], [\mathbb{D}^z_n]\right\}$$

Proof. By theorem 3.5.2 we deduce that the classes in the clips $[\mathbb{D}^z_n] \circledcirc [\mathrm{SO}(2) \oplus \mathbb{Z}^c_2]$ are in the following list

$$\left\{[\mathbb{1}], [\mathbb{Z}^-_2], [\mathbb{Z}_n]\right\}.$$

All the classes of the above list can be realized by a rotation g using the union $\mathbb{Z}_n \cap g\mathrm{SO}(2)g^{-1} \cup (-(\gamma\mathbb{Z}_n \cap g\mathrm{SO}(2)g^{-1}))$ (3.18) where $\mathrm{SO}(2)$ consists of all the rotations around $\boldsymbol{e}_3$. Indeed, we get:

- $[\mathbb{Z}^-_2]$ for a rotation g such that, $\exists i = 1, \ldots, n$, $g\boldsymbol{e}_3 = \mathbf{b}_i$,
- $[\mathbb{Z}_n]$ for the identity rotation for instance.

As for the classes in $[\mathbb{D}^z_n] \circledcirc [\mathrm{O}(2) \oplus \mathbb{Z}^c_2]$, by theorem 3.5.2 we know that such classes are in the following list

$$\left\{[\mathbb{1}], [\mathbb{Z}_{d_2}], [\mathbb{Z}^-_2], [\mathbb{D}^z_{d_2}], [\mathbb{D}^z_n]\right\}.$$

By the same reasoning, the above classes can be all realized except for $[\mathbb{Z}_{d_2}]$ using (3.18)

$$\mathbb{Z}_n \cap g\mathrm{O}(2)g^{-1} \cup (-(\gamma\mathbb{Z}_n \cap g\mathrm{O}(2)g^{-1}))$$

where $\gamma\mathbb{Z}_n = \{\mathbf{r}(\mathbf{b}_i, \pi), i = 1, \ldots, n\}$ and $g\mathrm{O}(2)g^{-1} = \{r(g\boldsymbol{e}_3, \theta), r(g\mathbf{b}, \pi), \mathbf{b} \in (xy) \text{ plan}\}$. Indeed, we get

- $[\mathbb{Z}^-_2]$ for a rotation g such that, $\exists i = 1, \ldots, 3$, $g\mathbf{b} = \mathbf{b}_i$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{2}\right)$ that turns only $\boldsymbol{e}_2$ to $\boldsymbol{e}_1$),
- $[\mathbb{D}^z_{d_2}]$ for $g = \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ for example,

- $[\mathbb{D}_n^z]$ for the identity rotation for example.

□

3.5.3 Clips with $\mathbb{D}_{2n}^d$

First we have (see section 3.1)

$$\mathbb{D}_{2n}^d = \mathbb{D}_n \cup (-\gamma \mathbb{D}_n), \quad \gamma = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{n}\right)$$

where we can write

$$\mathbb{D}_n = \left\{\mathbf{r}\left(\boldsymbol{e}_3, \frac{2k_1\pi}{n}\right), \mathbf{r}(\mathbf{b}_{2l+1}, \pi); \quad k_1 = 0, \ldots, n-1\right\} \tag{3.21}$$

$$-\gamma\mathbb{D}_n = \left\{-\mathbf{r}\left(\boldsymbol{e}_3, \frac{(2k_2+1)\pi}{n}\right), -\mathbf{r}(\mathbf{b}_{2l}, \pi); k_2 = 0, \ldots, n-1\right\} \tag{3.22}$$

with

$$\mathbf{b}_1 = \boldsymbol{e}_1 \text{ and } \mathbf{b}_l = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{n}\right)\mathbf{b}_{l-1}, \ l = 2, \ldots, n. \tag{3.23}$$

Lemma 3.5.13. *Let m, $n \geq 2$ be two integers and $d = \gcd(m, n)$. Then*

$$[\mathbb{D}_{2n}^d] \circledcirc [\mathbb{Z}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_{2d}^-]\} & \text{if } \frac{m}{d} \text{ even,} \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_d]\} & \text{if } m \text{ even and } \frac{m}{d} \text{ odd,} \\ \{[\mathbb{1}], [\mathbb{Z}_d]\} & \text{else.} \end{cases}$$

Proof. From (3.18) we have to consider intersection

$$\mathbb{D}_{2n}^d \cap (g\mathbb{Z}_m g^{-1} \oplus \mathbb{Z}_2^c) = (\mathbb{D}_n \cap g\mathbb{Z}_m g^{-1}) \cup (-(\gamma\mathbb{D}_n \cap g\mathbb{Z}_m g^{-1})) \quad \gamma = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{n}\right)$$

which can always reduce to $\mathbb{1}$. Otherwise we only have to consider three cases:

- $g\mathbf{e}_3 = \pm\mathbf{e}_3$ and we deduce intersection from lemma 3.5.3,
- $g\mathbf{e}_3 = \pm\mathbf{b}_{2l}$ for some l and intersection reduces to $\mathbb{Z}_2^-$ for m even,
- $g\mathbf{e}_3 = \pm\mathbf{b}_{2l+1}$ for some l and intersection reduces to $\mathbb{Z}_2$ for m even, and this concludes the proof.

□

Lemma 3.5.14. *Let m, $n \geq 2$ be two integers, $d = \gcd(m, n)$ and $d_2 = \gcd(2, n)$. Then*

$$[\mathbb{D}_{2n}^d] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_{d_2}], [\mathbb{Z}_2^-], [\mathbb{Z}_{2d}^-], [\mathbb{D}_2^z], [\mathbb{D}_{2d}^d]\} & \text{if } \frac{m}{d} \text{ is even,} \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{Z}_d], [\mathbb{D}_d], [\mathbb{D}_d^z]\} & \text{if } \frac{m}{d} \text{ is odd and } m \text{ is even,} \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_d], [\mathbb{D}_d], [\mathbb{D}_d^z]\} & \text{else.} \end{cases}$$

Proof. We apply theorem 3.5.2 with $\Gamma_+ = \mathbb{D}_n$ and $\tilde{\Gamma} = \mathbb{D}_{2n}$. We deduce from [86, table 1]

$$[\mathbb{D}_n] \circledcirc [\mathbb{D}_m] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2](\text{if } m \text{ and } n \text{ even}), [\mathbb{Z}_d], [\mathbb{D}_d]\}$$

and

$$[\mathbb{D}_{2n}] \circledcirc [\mathbb{D}_m] = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{Z}_{2d}], [\mathbb{D}_{2d}]\} & \text{if } \frac{m}{d} \text{ even} \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{Z}_d], [\mathbb{D}_d]\} & \text{if } m \text{ even and } \frac{m}{d} \text{ odd} \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_d], [\mathbb{D}_d]\} & \text{if } m \text{ odd} \end{cases}$$

Hence, the classes in $[\mathbb{D}_n^z] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{D}_n] \circledcirc [\mathbb{D}_m]) \cap ([\mathbb{D}_{2n}] \circledcirc [\mathbb{D}_m]) = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2]\} & \text{if } \frac{m}{d} \text{ even,} \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{Z}_d], [\mathbb{D}_d]\} & \text{if } m \text{ even and } \frac{m}{d} \text{ odd,} \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_d], [\mathbb{D}_d]\} & \text{if } m \text{ odd,} \end{cases}$$

and the classes corresponding to type III subgroups are in the set

$$\begin{cases} \left\{[\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{Z}_{2d}^-], [\mathbb{D}_{2d}^z]\right\} & \text{if } \frac{m}{d} \text{ even,} \\ \left\{[\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{D}_d^z]\right\} & \text{if } m \text{ even and } \frac{m}{d} \text{ odd,} \\ \left\{[\mathbb{Z}_2^-], [\mathbb{D}_d^z]\right\} & \text{if } m \text{ odd.} \end{cases}$$

We can check that all the eventualities can occur by using (3.18):

$$(\mathbb{D}_n \cap g\mathbb{D}_m g^{-1}) \cup (-(\gamma\mathbb{D}_n \cap g\mathbb{D}_m g^{-1}))$$

where $\mathbb{D}_n$ and $\gamma\mathbb{D}_n$ are given in (3.22). We obtain

- $[\mathbb{D}_{2d}^d]$ if $\frac{m}{d}$ is even and $[\mathbb{D}_d]$ otherwise for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{e}_3$ and $g\mathbf{b}_i = \pm\mathbf{b}_{2l+1}$ for some l,

- $[\mathbb{D}_{2d}^d]$ if $\frac{m}{d}$ is even and $[\mathbb{D}_d^z]$ otherwise for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{e}_3$ and $g\mathbf{b}_i = \pm\mathbf{b}_{2l}$ for some l,

- $[\mathbb{Z}_{2d}^-]$ if $\frac{m}{d}$ is even and $[\mathbb{Z}_d]$ otherwise for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{e}_3$ only,

- $\begin{cases} [\mathbb{D}_2] & \text{if } m \text{ and } n \text{ even,} \\ [\mathbb{D}_2^z] & \text{if } m \text{ even and } n \text{ odd,} \\ [\mathbb{Z}_2] & \text{if } m \text{ odd and } n \text{ even,} \\ [\mathbb{Z}_2^-] & \text{if } m \text{ and } n \text{ odds,} \end{cases}$ for a rotation g such that $g\boldsymbol{e}_3 = \pm\mathbf{b}_{2l+1}$ for some l,

- $[\mathbb{Z}_2]$ for a rotation g such that $g\boldsymbol{e}_3 = \pm\mathbf{b}_{2l+1}$ for some l,

- $\begin{cases} [\mathbb{D}_2^z] & \text{if } m \text{ even,} \\ [\mathbb{Z}_2] & \text{if } m \text{ odd and } n \text{ even,} \\ [\mathbb{Z}_2^-] & \text{if } m \text{ and } n \text{ odds,} \end{cases}$ for a rotation g such that $g\boldsymbol{e}_3 = \mathbf{b}_{2l}$ and $g\mathbf{b}_i = \boldsymbol{e}_3$,

- $[\mathbb{Z}_2^-]$ if m is even for a rotation g such that $g\boldsymbol{e}_3 = \mathbf{b}_{2l}$.

□

Lemma 3.5.15. *For any integer $n \geq 2$ and $d_k = gcd(n,k)$ for $k = 2,3$, we have*

$$[\mathbb{D}_{2n}^d] \circledcirc [\mathbb{T} \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3}], [\mathbb{D}_{d_2}], [\mathbb{Z}_2^-], [\mathbb{D}_2^z]\right\}.$$

Proof. We deduce from [86, table 1] and theorem 3.5.2 that the classes in $[\mathbb{D}_{2n}^d] \circledcirc [\mathbb{T} \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{D}_n] \circledcirc [\mathbb{T}]) \cap ([\mathbb{D}_{2n}] \circledcirc [\mathbb{T}]) = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3}], [\mathbb{D}_{d_2}]\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}_2^-], [\mathbb{D}_2^z]\right\}.$$

We can check that all the eventualities can occur by using (3.18):

$$(\mathbb{D}_n \cap g\mathbb{T}g^{-1}) \cup (-(\gamma\mathbb{D}_n \cap g\mathbb{T}g^{-1})),$$

where $\mathbb{D}_n$ and $\gamma\mathbb{D}_n$ are given in (3.10) and (3.22) and $\mathbb{T}$ in (3.11). We get

- $[\mathbb{Z}_{d_3}]$ for a rotation g such that $g\boldsymbol{s}_{t_j} = \pm\boldsymbol{e}_3$,
- $[\mathbb{Z}_2]$ for a rotation g such that $g\boldsymbol{e}_i = \mathbf{b}_{2l+1}$ for $i = 1,\ldots,3$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{2l}\right)$),
- $[\mathbb{Z}_2^-]$ for a rotation g such that $g\boldsymbol{e}_i = \mathbf{b}_{2l}$ for $i = 1,\ldots 3$,
- $[\mathbb{D}_{d_2}]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{e}_3$ for $i = 1,2,3$ and the two remaining $\boldsymbol{e}_i$ turn to two $\mathbf{b}_{2l+1}$ for some l,
- $[\mathbb{D}_{d_2}^z]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{e}_3$ for $i = 1,2,3$ and the two remaining $\boldsymbol{e}_i$ turn to two $\mathbf{b}_{2l}$ for some l.

□

Lemma 3.5.16. *Let n be any integer and $d_k = gcd(n,k)$ for $k = 2,3$, we have*

$$[\mathbb{D}_{2n}^d] \circledcirc [\mathbb{O} \oplus \mathbb{Z}_2^c] = \begin{cases} \left\{\mathsf{L}_{\mathbb{O}}, [\mathbb{Z}_4^-], [\mathbb{Z}_4], [\mathbb{D}_4], [\mathbb{D}_4^z]\right\} & \textit{if } 4|n, \\ \left\{\mathsf{L}_{\mathbb{O}}, [\mathbb{Z}_4^-], [\mathbb{D}_4^d]\right\} & \textit{if } n \textit{ is even and } 4 \nmid n, \\ \{\mathsf{L}_{\mathbb{O}}\} & \textit{if } n \textit{ is odd.} \end{cases}$$

$$\mathsf{L}_{\mathbb{O}} := [\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_{d_2}], [\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{Z}_{d_3}], [\mathbb{D}_{d_3}], [\mathbb{D}_{d_3}^z]$$

Proof. We deduce from [86, table 1]

$$[\mathbb{D}_n] \circledcirc [\mathbb{O}] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_4}], [\mathbb{D}_{d_2}], [\mathbb{D}_{d_3}], [\mathbb{D}_{d_4}]\}$$

where $d_4 = gcd(4, n)$ and

$$[\mathbb{D}_{2n}] \circledcirc [\mathbb{O}] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{2d_2}], [\mathbb{D}_2], [\mathbb{D}_{d_3}], [\mathbb{D}_{2d_2}]\}\,.$$

We deduce, by theorem 3.5.2, that the classes in $[\mathbb{D}^d_{2n}] \circledcirc [\mathbb{O} \oplus \mathbb{Z}^c_2]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{D}_n] \circledcirc [\mathbb{O}]) \cap ([\mathbb{D}_{2n}] \circledcirc [\mathbb{O}]) = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3}], [\mathbb{D}_{d_2}], [\mathbb{D}_{d_3}], [\mathbb{Z}_4](\text{if } 4 \mid n), [\mathbb{D}_4](\text{if } 4 \mid n)\}$$

and the classes corresponding to type III subgroups are in

$$\left\{[\mathbb{Z}^-_2], [\mathbb{Z}^-_4](\text{ if } n \text{ is even}), [\mathbb{D}^z_2], [\mathbb{D}^z_{d_3}], [\mathbb{D}^z_4](\text{if } 4 \mid n), [\mathbb{D}^d_4](\text{if } n \text{ is even and } 4 \nmid n)\right\}.$$

We can check that all the eventualities can occur by using (3.18):

$$(\mathbb{D}_n \cap g\mathbb{O}g^{-1}) \cup (-(\gamma\mathbb{D}_n \cap g\mathbb{O}g^{-1}))$$

where $\mathbb{D}_n$ and $\gamma\mathbb{D}_n$ are given in (3.10) and (3.22) and $\mathbb{O}$ in (3.12). We get

- $[\mathbb{Z}_2]$ for a rotation g such that $g\boldsymbol{a}_{c_k} = \mathbf{b}_{2l+1}$ for $i = 1, \dots n$,
- $[\mathbb{D}_{d_2}]$ for a rotation g such that $g\boldsymbol{a}_{c_k} = \boldsymbol{e}_3$ and two other edge axes $\boldsymbol{a}_{c_k}$ turn to two orthogonal axes $\mathbf{b}_{2l+1}$ (exists for n even) for some l,
- $[\mathbb{Z}^-_2]$ for a rotation g such that $g\boldsymbol{a}_{c_k} = \mathbf{b}_{2l}$,
- $[\mathbb{D}^z_2]$ for a rotation g such that $g\boldsymbol{a}_{c_k} = \mathbf{b}_{2l+1}$ and two other edge axes $\boldsymbol{a}_{c_k}$ turn to two orthogonal axes $\mathbf{b}_{2l}$ for some l,
- $[\mathbb{Z}_{d_3}]$ for a rotation g such that $g\boldsymbol{s}_{t_j} = \boldsymbol{e}_3$,
- $[\mathbb{D}_{d_3}]$ or $[\mathbb{D}^z_{d_3}]$ for a rotation g such that $g\boldsymbol{s}_{t_j} = \boldsymbol{e}_3$ and three other edge axes $\boldsymbol{a}_{c_k}$ turn to three secondary axis of $\mathbb{D}_n$ (either three $\mathbf{b}_{2l+1}$ or three $\mathbf{b}_{2l}$) (one can take for instance $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{4}\right) \circ \mathbf{r}\left(< 1, -1, 0 >, \arccos\left(1/\sqrt{3}\right)\right)$ to get $\mathbb{D}_{d_3}$),
- $[\mathbb{Z}_4]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{e}_3$ for $i = 1, \dots, 3$ (when $4 \mid n$),
- $[\mathbb{Z}^-_4]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{e}_3$ for $i = 1, \dots, 3$ (when n is even and $4 \nmid n$),
- $[\mathbb{D}_4]$ or $[\mathbb{D}^z_4]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{e}_3$ with $4 \mid n$ and two edge axes $\boldsymbol{a}_{c_k}$ together with the remaining two $\boldsymbol{e}_i$ turn to four secondary axis of $\mathbb{D}_n$ (either four $\mathbf{b}_{2l+1}$ or four $\mathbf{b}_{2l}$),
- $[\mathbb{D}^d_4]$ for the identity rotation for instance.

□

Lemma 3.5.17. *For any integer $n \geq 2$ and $d_k = gcd(n,k)$ for $k = 2,3,5$, we have*

$$[\mathbb{D}^d_{2n}] \circledcirc [\mathbb{I} \oplus \mathbb{Z}^c_2] = \left\{[\mathbb{1}], [\mathbb{Z}^-_2], [\mathbb{Z}_2], [\mathbb{D}_{d_2}], [\mathbb{D}^z_2], [\mathbb{Z}_{d_3}], [\mathbb{Z}_{d_5}]\right\}$$

Proof. We deduce from [86, table 1] and theorem 3.5.2 that the classes in $[\mathbb{D}^d_{2n}] \circledcirc [\mathbb{I} \oplus \mathbb{Z}^c_2]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{D}_n] \circledcirc [\mathbb{I}]) \cap ([\mathbb{D}_{2n}] \circledcirc [\mathbb{I}]) = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_{d_2}], [\mathbb{Z}_{d_3}], [\mathbb{D}^z_{d_3}], [\mathbb{Z}_{d_5}], [\mathbb{D}^z_{d_5}]\right\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}^-_2], [\mathbb{D}^z_2], [\mathbb{D}^z_{d_3}], [\mathbb{D}^z_{d_5}]\right\}.$$

We can check that all the eventualities can occur except $[\mathbb{D}_{d_3}]$, $[\mathbb{D}^z_{d_3}]$, $[\mathbb{D}_{d_5}]$, $[\mathbb{D}^z_{d_5}]$ for the same argument as in lemma 3.5.11 by using (3.18):

$$(\mathbb{D}_n \cap g\mathbb{I}g^{-1}) \cup (-(\gamma\mathbb{D}_n \cap g\mathbb{I}g^{-1}))$$

where $\mathbb{D}_n$ and $\gamma\mathbb{D}_n$ are given in (3.10) and (3.22) and $\mathbb{I}$ in (3.14). We get

- $[\mathbb{Z}^-_2]$ for a rotation g such that $g\boldsymbol{w}_k = \mathbf{b}_{2l}$ for $k = 1, \ldots, 15$,
- $[\mathbb{Z}_2]$ for a rotation g such that $g\boldsymbol{w}_k = \mathbf{b}_{2l+1}$ for $k = 1, \ldots, 15$,
- $[\mathbb{D}_{d_2}]$ for a rotation g such that $g\boldsymbol{w}_k = \boldsymbol{e}_3$ and two other axes $\boldsymbol{w}_k$ turn to two orthogonal axes $\mathbf{b}_{2l+1}$,
- $[\mathbb{D}^z_{d_2}]$ for a rotation g such that $g\boldsymbol{w}_k = \boldsymbol{e}_3$ and two other axes $\boldsymbol{w}_k$ turn to two orthogonal axes $\mathbf{b}_{2l}$,
- $[\mathbb{Z}_{d_3}]$ for a rotation g such that $g\boldsymbol{v}_j = \boldsymbol{e}_3$ for $j = 1, \ldots, 10$,
- $[\mathbb{Z}_{d_5}]$ for a rotation g such that $g\boldsymbol{u}_i = \boldsymbol{e}_3$ for $i = 1, \ldots, 6$.

□

Finally, we have

Lemma 3.5.18. *For any integer $n \geq 2$ we have*

$$[\mathbb{D}^d_{2n}] \circledcirc [\mathrm{SO}(2) \oplus \mathbb{Z}^c_2] = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}^-_2], [\mathbb{Z}^-_{2n}]\right\}$$
$$[\mathbb{D}^d_{2n}] \circledcirc [\mathrm{O}(2) \oplus \mathbb{Z}^c_2] = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}^-_2], [\mathbb{D}_{d_2}], [\mathbb{D}^z_2], [\mathbb{D}^d_{2n}]\right\}.$$

Proof. By theorem 3.5.2 we deduce that the classes in the clips $[\mathbb{D}^d_{2n}] \circledcirc [\mathrm{SO}(2) \oplus \mathbb{Z}^c_2]$ are in the following list

$$\left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}^-_2], [\mathbb{Z}^-_{2n}]\right\}.$$

All the classes of the above list can be realized by a rotation g using the union

$$\mathbb{D}_n \cap g\mathrm{SO}(2)g^{-1} \cup (-(\gamma\mathbb{D}_n \cap g\mathrm{SO}(2)g^{-1}))(3.18).$$

Indeed, we get:

- $[\mathbb{Z}_2]$ for a rotation g such that $g\boldsymbol{e}_3 = \mathbf{b}_{2l+1}$,
- $[\mathbb{Z}_2^-]$ for a rotation g such that $g\boldsymbol{e}_3 = \mathbf{b}_{2l}$,
- $[\mathbb{Z}_{2n}^-]$ for the identity rotation for instance.

As for the classes in $[\mathbb{D}_{2n}^d] \circledcirc [\mathrm{O}(2) \oplus \mathbb{Z}_2^c]$, by theorem 3.5.2 we know that such classes are in the following list

$$\left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_{d_2}], [\mathbb{D}_{2n}^d], [\mathbb{D}_2^z]\right\}.$$

By the same reasoning, the above classes can be all realized by a rotation g using (3.18)

$$\mathbb{D}_n \cap g\mathrm{O}(2)g^{-1} \cup (-(\gamma\mathbb{D}_n \cap g\mathrm{O}(2)g^{-1}))$$

where $g\mathrm{O}(2)g^{-1} = \{r(g\boldsymbol{e}_3, \theta), r(g\mathbf{b}, \pi), \mathbf{b} \in xy \text{ plane}\}$. We get,

- $[\mathbb{Z}_2]$ for a rotation g such that $g = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ that turns only $\boldsymbol{e}_3$ to $\boldsymbol{e}_1$ for instance,
- $[\mathbb{Z}_2^-]$ for a rotation g such that $g\mathbf{b} = \mathbf{b}_{2k}$ for some k and some $\mathbf{b} \in (xy)$-plane and that does not turn $\boldsymbol{e}_3$ to the other axes of $\mathbb{D}_{2n}$ (take for instance $g = \mathbf{r}\left(\mathbf{b}_{2k}, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, \alpha\right)$ where α is the angle between $\mathbf{b}$ and $\mathbf{b}_{2k}$),
- $[\mathbb{D}_{d_2}]$ for a rotation $g = \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ for instance (for n even there exists k such that $\mathbf{b}_{2k+1} = \boldsymbol{e}_2$),
- $[\mathbb{D}_2^z]$ for a rotation $g = \mathbf{r}\left(\boldsymbol{v}, \frac{\pi}{2}\right)$ where $\boldsymbol{v}$ is a secondary axis of $\mathbb{D}_{2n}$ orthogonal to $\boldsymbol{e}_3$ and $\mathbf{b}_{2k}$ for instance,
- $[\mathbb{D}_{2n}^d]$ for the identity rotation for example.

□

3.5.4 Clips with $\mathbb{O}^-$

First, we introduce a useful decomposition of the subgroup $\mathbb{O}^-$ (see section 3.1), constructed from the couple $(\mathbb{T}, \mathbb{O})$ of index 2

$$\mathbb{O}^- = \mathbb{T} \cup (-\gamma\mathbb{T}), \quad \gamma = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{2}\right)$$

where

$$\mathbb{T} = \bigcup_{i=1}^{3} \mathbb{Z}_2^{\boldsymbol{e}_i} \bigcup_{j=1}^{4} \mathbb{Z}_3^{\boldsymbol{s}_{t_j}}, \tag{3.24}$$

$$\gamma\mathbb{T} = \left\{\mathbf{r}\left(\boldsymbol{a}_{c_k}, \pi\right), \mathbf{r}\left(\boldsymbol{e}_i, \frac{\pi}{2}\right), \mathbf{r}\left(\boldsymbol{e}_i, \frac{3\pi}{2}\right)\right\}. \tag{3.25}$$

Lemma 3.5.19. *Let $m \geq 2$ be an integer and $d_k' = \gcd(k, m)$ $(k = 2, 3)$. Then we have*

$$[\mathbb{O}^-] \circledcirc [\mathbb{Z}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \left\{[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{Z}_{d_3'}], [\mathbb{Z}_4^-]\right\} & \text{if } 4|m, \\ \left\{[\mathbb{1}], [\mathbb{Z}_{d_2'}], [\mathbb{Z}_{d_2'}^-], [\mathbb{Z}_{d_3'}]\right\} & \text{otherwise.} \end{cases}$$

Proof. From (3.18) we have to consider intersection

$$\mathbb{O}^- \cap (g\mathbb{Z}_m g^{-1} \oplus \mathbb{Z}_2^c) = (\mathbb{T} \cap g\mathbb{Z}_m g^{-1}) \cup (-(\gamma\mathbb{T} \cap g\mathbb{Z}_m g^{-1})) \quad \gamma = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{n}\right)$$

which can always reduce to $\mathbb{1}$. Otherwise we only have to consider three cases:

- $g\boldsymbol{e}_3 = \pm\boldsymbol{e}_i$ and we get $[\mathbb{Z}_4^-]$ if $4 \mid m$ and $[\mathbb{Z}_{d_2'}]$ if not,
- $g\boldsymbol{e}_3 = \pm\boldsymbol{s}_{t_j}$ and we get $[\mathbb{Z}_{d_3'}]$,
- $g\boldsymbol{e}_3 = \pm\boldsymbol{a}_{c_k}$ and we get $[\mathbb{Z}_{d_2'}^-]$.

□

Lemma 3.5.20. *Let $m \geq 2$ be an integer. We have*

$$[\mathbb{O}^-] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_{d_3'}], [\mathbb{D}_{d_3'}^z], [\mathbb{Z}_4^-], [\mathbb{D}_2^z], [\mathbb{D}_4^d]\right\} & \textit{if } 4|m, \\ \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_{d_3'}], [\mathbb{D}_{d_3'}^z], [\mathbb{D}_2], [\mathbb{D}_2^z]\right\} & \textit{if } m \textit{ is even and } 4 \nmid m, \\ \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_{d_3'}], [\mathbb{D}_{d_3'}^z]\right\} & \textit{if } m \textit{ is odd.} \end{cases}$$

Proof. We apply theorem 3.5.2 with $\Gamma_+ = \mathbb{T}$ and $\tilde{\Gamma} = \mathbb{O}$. We deduce from [86, table 1]

$$[\mathbb{T}] \circledcirc [\mathbb{D}_m] = \left\{[\mathbb{1}], [\mathbb{Z}_{d_2'}], [\mathbb{Z}_{d_3'}], [\mathbb{D}_{d_2'}]\right\}$$

and

$$[\mathbb{O}] \circledcirc [\mathbb{D}_m] = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3'}], [\mathbb{Z}_{d_4'}], [\mathbb{D}_{d_2'}], [\mathbb{D}_{d_3'}], [\mathbb{D}_{d_4'}]\right\}.$$

Hence, the classes in $[\mathbb{O}^-] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{T}] \circledcirc [\mathbb{D}_m]) \cap ([\mathbb{O}] \circledcirc [\mathbb{D}_m]) = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_{d_3'}], [\mathbb{D}_{d_2'}]\right\}$$

and the classes corresponding to type III subgroups are in

$$\begin{cases} \left\{[\mathbb{Z}_2^-], [\mathbb{D}_4^d], [\mathbb{Z}_4^-], [\mathbb{D}_2^z], [\mathbb{D}_{d_3'}^z]\right\} & \text{if } 4 \mid m, \\ \left\{[\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{D}_{d_3'}]\right\} & \text{if } m \text{ even and } 4 \nmid m, \\ \left\{[\mathbb{Z}_2^-], [\mathbb{D}_{d_3'}^z]\right\} & \text{if } m \text{ odd.} \end{cases}$$

We can check that all the eventualities can occur by using (3.18), except $[\mathbb{D}_2]$ when $4 \mid m$ since it becomes $\mathbb{D}_4^d$ in this case. Consider

$$(\mathbb{T} \cap g\mathbb{D}_m g^{-1}) \cup (-(\gamma\mathbb{T} \cap g\mathbb{D}_m g^{-1}))$$

where $\gamma\mathbb{T}$ is given by (3.25). We obtain

- $[\mathbb{Z}_2]$ for a rotation g such that $g\mathbf{b}_i = \boldsymbol{e}_j$ for $i = 1, \ldots, m$ and $j = 1, \ldots, 3$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{2}\right)$),
- $[\mathbb{Z}_2^-]$ for a rotation g such that $g\mathbf{b}_i = \boldsymbol{a}_{c_k}$ for $i = 1, \ldots, m$ (take for instance $g = \mathbf{r}\left(\boldsymbol{a}_{c_k}, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{4}\right)$),

- $[\mathbb{Z}_{d'_3}]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{s}_{t_j}$,
- $[\mathbb{D}^z_{d'_3}]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{s}_{t_j}$ and three secondary axis $\mathbf{b}_i$ of $\mathbb{D}_m$ turn to three $\boldsymbol{a}_{c_k}$,
- $[\mathbb{D}_2]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{e}_i$ and two orthogonal secondary axis of $\mathbb{D}_m$ turn to the two remaining $\boldsymbol{e}_i$ and that is possible when m is even and $4 \nmid m$ since if $4 \mid m$ we get $[\mathbb{D}^d_4]$,
- $[\mathbb{D}^z_2]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{e}_i$ and two orthogonal secondary axis of $\mathbb{D}_m$ turn to orthogonal $\boldsymbol{a}_{c_k}$ and this is possible if m is even,
- $[\mathbb{Z}^-_4]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{e}_i$ for $i = 1, \ldots, 3$ and if $4 \mid m$.

□

Lemma 3.5.21. *We have*

$$[\mathbb{O}^-] \circledcirc [\mathbb{T} \oplus \mathbb{Z}^c_2] = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}^-_2], [\mathbb{D}_2], [\mathbb{D}^z_2], [\mathbb{Z}_3], [\mathbb{T}]\right\}.$$

Proof. We deduce from [86, table 1] and theorem 3.5.2 that the classes in $[\mathbb{O}^-] \circledcirc [\mathbb{T} \oplus \mathbb{Z}^c_2]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{T}] \circledcirc [\mathbb{T}]) \cap ([\mathbb{O}] \circledcirc [\mathbb{T}]) = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{D}_2], [\mathbb{T}]\}$$

and the classes corresponding to type III subgroups are in

$$\left\{[\mathbb{Z}^-_2], [\mathbb{D}^z_2]\right\}.$$

We can check that all the eventualities can occur by using (3.18):

$$(\mathbb{T} \cap g\mathbb{T}g^{-1}) \cup (-(\gamma\mathbb{T} \cap g\mathbb{T}g^{-1})),$$

where $\gamma\mathbb{T}$ is given by (3.25) and $\mathbb{T}$ in (3.11). We get

- $[\mathbb{Z}_3]$ for a rotation g such that $g\boldsymbol{s}_{t_j} = \boldsymbol{s}_{t_l}$,
- $[\mathbb{D}_2]$ for a rotation $g = \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ for instance,
- $[\mathbb{Z}_2]$ for a rotation $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ for instance,
- $[\mathbb{D}^z_2]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{e}_j$ for $i = 1, \ldots, 3$ and the two remaining $\boldsymbol{e}_i$ turn to two $\boldsymbol{a}_{c_k}$ (for instance $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{4}\right)$),
- $[\mathbb{Z}^-_2]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{a}_{c_k}$ for $i = 1, \ldots 3$ (for instance $g = \mathbf{r}\left(\boldsymbol{a}_{c_1}, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{2}\right)$),
- $[\mathbb{T}]$ for the identity rotation for instance.

□

Lemma 3.5.22. *We have*

$$[\mathbb{O}^-] \circledcirc [\mathbb{O} \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_3], [\mathbb{Z}_4^-], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{D}_4^d], [\mathbb{O}^-]\right\}.$$

Proof. We deduce, by theorem 3.5.2, that the classes in $[\mathbb{O}^-] \circledcirc [\mathbb{O} \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{T}] \circledcirc [\mathbb{O}]) \cap ([\mathbb{O}] \circledcirc [\mathbb{O}]) = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{D}_2], [\mathbb{T}]\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}_2^-], [\mathbb{Z}_4^-], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{D}_4^d], [\mathbb{O}^-]\right\}.$$

We can check that all the eventualities can occur by using (3.18) except $[\mathbb{D}_2]$ since to get $[\mathbb{D}_2]$ we need a rotation g such that $g\boldsymbol{a}_{c_k} = \boldsymbol{e}_i$ and $g\boldsymbol{e}_i = \boldsymbol{e}_i$ which will give $[\mathbb{Z}_4^-]$. We have

$$(\mathbb{T} \cap g\mathbb{O}g^{-1}) \cup (-(\gamma\mathbb{T} \cap g\mathbb{O}g^{-1}))$$

where $\gamma\mathbb{T}$ is given by (3.25) and $\mathbb{O}$ in (3.12):

- $[\mathbb{Z}_2]$ for a rotation g such that $g\boldsymbol{a}_{c_k} = \boldsymbol{e}_i$ for $i = 1, \ldots, 3$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_1, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, -\frac{\pi}{4}\right)$),
- $[\mathbb{Z}_2^-]$ for a rotation $g = \mathbf{r}\left(\boldsymbol{a}_{c_1}, \frac{\pi}{3}\right) \circ \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{2}\right)$,
- $[\mathbb{D}_2^z]$ for a rotation $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{2}\right)$ for example,
- $[\mathbb{Z}_3]$ for a rotation g such that $g\boldsymbol{s}_{t_j} = \boldsymbol{s}_{t_l}$,
- $[\mathbb{D}_{d_3}^z]$ for a rotation g such that $g\boldsymbol{s}_{t_j} = \boldsymbol{s}_{t_l}$ and three edge axes $\boldsymbol{a}_{c_k}$ turn to three $\boldsymbol{a}_{c_k}$,
- $[\mathbb{Z}_4^-]$ for a rotation g such that $g\boldsymbol{e}_i = \boldsymbol{e}_j$ for some $i, j = 1, \ldots, 3$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{3}\right)$),
- $[\mathbb{D}_4^d]$ for a rotation $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{2}\right)$ for example,
- $[\mathbb{O}^-]$ for the identity rotation for instance.

□

Lemma 3.5.23. *We have*

$$[\mathbb{O}^-] \circledcirc [\mathbb{I} \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{Z}_3], [\mathbb{D}_2^z], [\mathbb{T}]\right\}.$$

Proof. We deduce from [86, table 1] and theorem 3.5.2 that the classes in $[\mathbb{O}^-] \circledcirc [\mathbb{I} \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathbb{T}] \circledcirc [\mathbb{I}]) \cap ([\mathbb{O}] \circledcirc [\mathbb{I}]) = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{T}]\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{D}_3^z]\right\}.$$

We can check that all the eventualities can occur except $[\mathbb{D}_3^z]$ (same argument as in lemma 3.5.11) by using (3.18):

$$(\mathbb{T} \cap g\mathbb{I}g^{-1}) \cup (-(\gamma\mathbb{T} \cap g\mathbb{I}g^{-1}))$$

where $\gamma\mathbb{T}$ is given by (3.25) and $\mathbb{I}$ in (3.14). Hence, we get

- $[\mathbb{Z}_2]$ for a rotation g such that $g\boldsymbol{w}_k = \boldsymbol{e}_i$ for $k = 1, \ldots, 15$ and $i = 1, \ldots, 3$,
- $[\mathbb{Z}_2^-]$ for a rotation g such that $g\boldsymbol{w}_k = \boldsymbol{a}_{c_k}$,
- $[\mathbb{D}_2^z]$ for a rotation g such that $g\boldsymbol{w}_k = \boldsymbol{e}_i$ and two other axes $\boldsymbol{w}_k$ turn to two orthogonal axes $\boldsymbol{a}_{c_k}$ (take for instance $g = \mathbf{r}\left(\boldsymbol{e}_3, \frac{\pi}{4}\right)$),
- $[\mathbb{Z}_3]$ for a rotation g such that $g\boldsymbol{v}_j = \boldsymbol{s}_{t_j}$,
- $[\mathbb{T}]$ for the identity rotation for instance.

□

Lemma 3.5.24. *We have*

$$[\mathbb{O}^-] \circledcirc [\mathrm{SO}(2) \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_3], [\mathbb{Z}_2^-], [\mathbb{Z}_4^-]\right\}.$$

Proof. By theorem 3.5.2 we deduce that the classes in the clips $[\mathbb{O}^-] \circledcirc [\mathrm{SO}(2) \oplus \mathbb{Z}_2^c]$ are in the following list

$$\left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{Z}_2^-], [\mathbb{Z}_4^-]\right\}.$$

All the classes of the above list can be realized by a rotation g using the union $\mathbb{T} \cap g\mathrm{SO}(2)g^{-1} \cup (-(\gamma\mathbb{T} \cap g\mathrm{SO}(2)g^{-1}))$ (3.18) except $[\mathbb{Z}_2]$. Indeed, we get:

- $[\mathbb{Z}_3]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{s}_{t_j}$,
- $[\mathbb{Z}_2^-]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{a}_{c_k}$,
- $[\mathbb{Z}_4^-]$ for the identity rotation for instance.

□

Lemma 3.5.25. *We have*

$$[\mathbb{O}^-] \circledcirc [\mathrm{O}(2) \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{D}_3^z], [\mathbb{D}_4^d]\right\}.$$

Proof. By theorem 3.5.2 we deduce that the classes in the clips $[\mathbb{O}^-] \circledcirc [\mathrm{O}(2) \oplus \mathbb{Z}_2^c]$ are in the following list

$$\left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{D}_4^d]\right\}.$$

Using the union $\mathbb{T} \cap g\mathrm{O}(2)g^{-1} \cup (-(\gamma\mathbb{T} \cap g\mathrm{O}(2)g^{-1}))$ (3.18) where $g\mathrm{O}(2)g^{-1} = \{r(g\boldsymbol{e}_3, \theta), r(g\mathbf{b}, \pi), \mathbf{b} \in xy \text{ plan}\}$, we deduce the classes that can be realized by a rotation g:

- $[\mathbb{Z}_2^-]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{a}_{c_k}$,
- $[\mathbb{D}_3^z]$ for a rotation g such that $g\boldsymbol{e}_3 = \boldsymbol{s}_{t_j}$ and three axes $\mathbf{b}$ of the (xy)-plane turn to $\boldsymbol{a}_{c_k}$ (take for instance $g = \mathbf{r}\left(< -1, 1, 0 >, \arccos\left(\frac{1}{\sqrt{3}}\right)\right)$),
- $[\mathbb{D}_4^d]$ for the identity rotation for instance.

□

3.5.5 Clips with $\mathrm{O}(2)^-$

We construct $\mathrm{O}(2)^-$ as follows

$$\begin{aligned}\mathrm{O}(2)^- &= \mathrm{SO}(2) \cup -(\gamma \mathrm{SO}(2)) \quad \text{where } \gamma = \mathbf{r}(\boldsymbol{e}_1, \pi) \\ &= \{\mathbf{r}(\boldsymbol{e}_3, \theta), \theta \in [0, 2\pi], -\mathbf{r}(\mathbf{b}, \pi)\}\,.\end{aligned}$$

where $\mathbf{r}(\mathbf{b}, \pi)$ represent the symmetry with respect to all the axes in the xy plane.

Lemma 3.5.26. *Let $m \geq 2$ be an integer and $d_2' = \gcd(2, m)$. We have*

$$[\mathrm{O}(2)^-] \circledcirc [\mathbb{Z}_m \oplus \mathbb{Z}_2^c] = \left\{[\mathbb{1}], [\mathbb{Z}_m], [\mathbb{Z}_{d_2'}^-]\right\}.$$

Proof. We get the result by considering the following intersection (from (3.18))

$$\mathrm{O}(2)^- \cap (g\mathbb{Z}_m g^{-1} \oplus \mathbb{Z}_2^c) = (\mathrm{SO}(2) \cap g\mathbb{Z}_m g^{-1}) \cup (-(\gamma \mathrm{SO}(2) \cap g\mathbb{Z}_m g^{-1}))$$

where $\gamma = \mathbf{r}(\boldsymbol{e}_1, \pi)$ and $\gamma\mathrm{SO}(2) = \{\mathbf{r}(\mathbf{b}, \pi)\}$. □

The proof of the following lemma is similar to the proof of lemma 3.5.8.

Lemma 3.5.27. *For any integer $m \geq 2$, we have*

$$[\mathrm{O}(2)^-] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c] = \begin{cases} \{[\mathbb{1}], [\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{D}_m^z]\} & \textit{if } m \textit{ is even,} \\ \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_m^z]\} & \textit{if } m \textit{ is odd.} \end{cases}$$

Proof. We apply theorem 3.5.2 with $\Gamma_+ = \mathrm{SO}(2)$ and $\tilde{\Gamma} = \mathrm{O}(2)$. We deduce from [86, table 1]

$$[\mathrm{SO}(2)] \circledcirc [\mathbb{D}_m] = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_m]\}$$

and

$$[\mathrm{O}(2)] \circledcirc [\mathbb{D}_m] = \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_{d_2'}], [\mathbb{D}_m]\right\}.$$

Hence, the classes in $[\mathrm{O}(2)^-] \circledcirc [\mathbb{D}_m \oplus \mathbb{Z}_2^c]$, corresponding to type I subgroups, are in the following list

$$([\mathrm{SO}(2)] \circledcirc [\mathbb{D}_m]) \cap ([\mathrm{O}(2)] \circledcirc [\mathbb{D}_m]) = \{[\mathbb{1}], [\mathbb{Z}_2]\}$$

and the classes corresponding to type III subgroups are in the set

$$\left\{[\mathbb{Z}_2^-], [\mathbb{D}_{d_2'}^z], [\mathbb{D}_m^z]\right\}.$$

We can check that all the eventualities can occur by using (3.18), except $[\mathbb{D}_2]$ when $4 \mid m$ since it becomes $\mathbb{D}_4^d$ in this case. Consider

$$(\mathrm{SO}(2) \cap g\mathbb{D}_m g^{-1}) \cup (-(\gamma\mathrm{SO}(2) \cap g\mathbb{D}_m g^{-1}))$$

where $\gamma\mathrm{SO}(2) = \{\mathbf{r}(\mathbf{b}, \pi),\ \mathbf{b} \in xy \text{ plane}\}$. We obtain

- $[\mathbb{Z}_2]$ for a rotation g such that $g\mathbf{b}_i = \boldsymbol{e}_3$ (possible only if m is odd since if m is even the second part of the intersection will not be empty),
- $[\mathbb{Z}_2^-]$ for a rotation g such that $g\mathbf{b}_i = \mathbf{b}$ for some $\mathbf{b}$ in the xy plane,
- $[\mathbb{D}_{d_2'}^z]$ for a rotation $g = \mathbf{r}\left(\boldsymbol{e}_2, \frac{\pi}{2}\right)$ for example,
- $[\mathbb{D}_m^z]$ for the identity rotation for instance.

□

The argumentation for the calculation of the clips with $\mathrm{O}(2)^-$ is very similar to the ones for $\mathbb{D}_n^z$ exposed in subsection 3.5.2.

Lemma 3.5.28. *We have*

$$\begin{aligned}
[\mathrm{O}(2)^-] \circledcirc [\mathbb{T} \oplus \mathbb{Z}_2^c] &= \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{Z}_2^-], [\mathbb{D}_2^z]\right\}. \\
[\mathrm{O}(2)^-] \circledcirc [\mathbb{O} \oplus \mathbb{Z}_2^c] &= \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{D}_4^z]\right\}. \\
[\mathrm{O}(2)^-] \circledcirc [\mathbb{I} \oplus \mathbb{Z}_2^c] &= \left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_2^-], [\mathbb{D}_2^z]\right\}.
\end{aligned}$$

And finally we deduce the clips with $\mathrm{SO}(2) \oplus \mathbb{Z}_2^c$ and $\mathrm{O}(2) \oplus \mathbb{Z}_2^c$ in the same way as in lemma 3.5.12.

Lemma 3.5.29. *We have*

$$\begin{aligned}
[\mathrm{O}(2)^-] \circledcirc [\mathrm{SO}(2) \oplus \mathbb{Z}_2^c] &= \left\{[\mathbb{1}], [\mathbb{Z}_2^-], [\mathrm{SO}(2)]\right\}. \\
[\mathrm{O}(2)^-] \circledcirc [\mathrm{O}(2) \oplus \mathbb{Z}_2^c] &= \left\{[\mathbb{D}_2^z], [\mathrm{O}(2)^-]\right\}.
\end{aligned}$$

Chapter 4

Application to constitutive laws

An explicit set of 25 isotropy classes is deduced for the standard O(3)-representation on the coupled Piezoelectric law in three dimensions, where both elasticity tensor, piezoelectricity tensor and permittivity tensor occur. The result obtained in this chapter is contained in an article accepted for publication in *Mathematics and Mechanics of Complex Systems* ([5]).

4.1 Introduction to Piezoelectricity coupled law

In mechanics, constitutive laws relate the stress imposed on a material and the resulting deformation at a macroscopic level. They are used to describe the behavior of a material exposed to some constraints. These laws are modeled using tensors and the questions related to their symmetries can be formulated in the language of group representation theory. We propose here to apply clips operation to the specific case of the linear *Piezoelectricity law*. We introduce the space of constitutive tensors occurring in the mechanical description of Piezoelectricity, which describes the electrical behavior of a material subject to mechanical stress. It is defined by a triplet of tensors given by an elasticity tensor, a piezoelectricity tensor and a permittivity tensor. Such a space is naturally endowed with an O(3)-representation, and the finite set of isotropy classes is obtained in theorem 4.4.1 below.

We now recall the Piezoelectricity law (details can be found in [102, 64, 96, 75]). First, the mechanical state of a material is characterized by two symmetric second order tensors: the stress tensor $\boldsymbol{\sigma}$ and the infinitesimal strain tensor $\boldsymbol{\varepsilon}$. The relation between these two tensors forms the constitutive law that describes the mechanical behavior of a specific material. In linear elasticity, the relation is linear known as the generalized Hooke's law, given by

$$\boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\varepsilon}$$

where $\mathbf{E}$ is the elasticity tensor, a fourth order tensor having the following index symmetries

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}, \quad i, j, k, l \in \{1, 2, 3\}.$$

We define the associated space of elasticity tensors $\mathbb{E}\mathrm{la}$, which is a 21-dimensional vector space.

Similarly to the mechanical state, the electrical state of a material is described by two vector

fields: the electric displacement field $\boldsymbol{d}$ and the electric field $\boldsymbol{e}$. These two fields are related and the relation between them forms the constitutive law that describes the electrical behavior of a material. In the linear case, it is given by

$$\boldsymbol{d} = \mathbf{S}.\boldsymbol{e}$$

where the second order symmetric tensor $\mathbf{S}$ is called the *permittivity* tensor. We define $\mathbb{S}$ to be the vector space of the permittivity tensors, which is of dimension 6.

Finally, the Piezoelectricity law is given by the coupled law

$$\begin{cases} \boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\varepsilon} - \boldsymbol{e}.\mathbf{P} \\ \boldsymbol{d} = \mathbf{P} : \boldsymbol{\sigma} + \mathbf{S}.\boldsymbol{e} \end{cases} .$$

In components (using Einstein notation), we write

$$\begin{cases} \sigma_{ij} = E_{ijkl}\varepsilon_{kl} - e_k P_{kij} \\ d_i = P_{ijk}\sigma_{jk} + S_{ij}e_j \end{cases} , \quad i,j,k,l \in \{1,2,3\}$$

which involves a third order tensor $\mathbf{P}$ called the *piezoelectricity* tensor, satisfying the index symmetry

$$P_{ijk} = P_{ikj}, \quad i,j,k \in \{1,2,3\}.$$

The vector space of piezoelectricity tensors is an 18 dimensional vector space, noted $\mathbb{P}\mathrm{iez}$.

As a consequence, the linear electromechanical behavior of any homogeneous material is defined by a triplet $\mathcal{P}$ of constitutive tensors

$$\mathcal{P} := (\mathbf{E}, \mathbf{P}, \mathbf{S}) \in \mathbb{E}\mathrm{la} \oplus \mathbb{P}\mathrm{iez} \oplus \mathbb{S}$$

and we define $\mathcal{P}\mathrm{iez}$ to be the space of Piezoelectricity constitutive tensors:

$$\mathcal{P}\mathrm{iez} = \mathbb{E}\mathrm{la} \oplus \mathbb{P}\mathrm{iez} \oplus \mathbb{S}.$$

The natural O(3)-representation ρ on $\mathcal{P}\mathrm{iez}$ is given in any orthonormal basis by

$$(\rho(g)\mathbf{E})_{ijkl} := g_{ip}g_{jq}g_{kr}g_{ls}E_{pqrs}, \quad (\rho(g)\mathbf{P})_{ijk} := g_{ip}g_{jq}g_{kr}P_{pqr}, \quad (\rho(g)\mathbf{S})_{ij} := g_{ip}g_{jq}S_{pq} \tag{4.1}$$

if $g \in \mathrm{O}(3)$ and $(\mathbf{E}, \mathbf{P}, \mathbf{S}) \in \mathcal{P}\mathrm{iez}$.

4.2 SO(3)-representation on the space of elasticity tensors

The elastic behavior of a material is represented by the elasticity tensor, the fourth order tensor $\mathbf{E}$ that relates the stress and strain tensors in the generalized Hooke law

$$\boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\varepsilon}$$

where $\boldsymbol{\sigma}$ is the stress tensor and $\boldsymbol{\varepsilon}$ is the strain tensor and the operation ":" is the contraction of two indices (for instance, $\mathbf{E} : \boldsymbol{\varepsilon}$ writes in components: $(\mathbf{E} : \boldsymbol{\varepsilon})_{ij} = E_{ijkl}\epsilon kl$).

4.2.1 Elasticity tensor

The main mechanical object in this study is the *elasticity tensor*

$$\mathbf{E} : \mathbb{S}^2(\mathbb{R}^3) \to \mathbb{S}^2(\mathbb{R}^3)$$

where $\mathbb{S}^2(\mathbb{R}^3)$ is the space of second order symmetric tensors on $\mathbb{R}^3$ (equipped with the canonical basis $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$) for which we consider the following orthonormal basis ($\mathbb{S}^2(\mathbb{R}^3) = \mathbb{R}^3 \otimes \mathbb{R}^3$)

$$\begin{aligned}
e_{11} &= \boldsymbol{e}_1 \otimes \boldsymbol{e}_1 \\
e_{22} &= \boldsymbol{e}_2 \otimes \boldsymbol{e}_2 \\
e_{33} &= \boldsymbol{e}_3 \otimes \boldsymbol{e}_3 \\
e_{23} &= \frac{1}{\sqrt{2}}(\boldsymbol{e}_2 \otimes \boldsymbol{e}_3 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_2) \\
e_{13} &= \frac{1}{\sqrt{2}}(\boldsymbol{e}_1 \otimes \boldsymbol{e}_3 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_1) \\
e_{12} &= \frac{1}{\sqrt{2}}(\boldsymbol{e}_1 \otimes \boldsymbol{e}_2 + \boldsymbol{e}_2 \otimes \boldsymbol{e}_1)
\end{aligned}$$

The elasticity tensor $\mathbf{E}$ is a contravariant fourth order tensor that takes a second order symmetric contravariant tensor $\boldsymbol{\sigma}$ and gives a second order symmetric covariant tensor $\boldsymbol{\varepsilon}$:

$$\sigma^{ij} = E^{ijkl}\varepsilon_{kl}. \tag{4.2}$$

Since we work in an orthonormal basis, we do not distinguish between contravariant and covariant tensors (we equip $\mathbb{R}^3$ with the usual scalar product), hence equation (4.2) becomes

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}.$$

In the orthonormal basis of $\mathbb{S}(\mathbb{R}^3)$ defined above, we write

$$\{\boldsymbol{\sigma}\} = \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sqrt{2}\sigma_{23} \\ \sqrt{2}\sigma_{13} \\ \sqrt{2}\sigma_{12} \end{pmatrix} \quad \text{and} \quad \{\boldsymbol{\varepsilon}\} = \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \sqrt{2}\varepsilon_{23} \\ \sqrt{2}\varepsilon_{13} \\ \sqrt{2}\varepsilon_{12} \end{pmatrix}$$

The symmetry of the tensors $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ induces an indicial symmetry in the first two indices i, j of E_{ijkl} as well as in the last two indices k, l. Moreover, the fact that $\mathbf{E}$ derives from a potential induces a major symmetry in the indices so that in the end $\mathbf{E}$ is endowed with the following

subscripts symmetries of its components (see [31, Chapter 3] or [67]),

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}.$$

We denote by $\mathbb{E}\mathrm{la}$ the space of elasticity tensors.

Thanks to these indicial symmetries, an elasticity tensor has 21 independent components and can be represented by a 6×6 symmetric matrix in the considered orthonormal basis of $\mathbb{S}(\mathbb{R}^2)$

$$\{\mathbf{E}\} = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & \sqrt{2}\,E_{1123} & \sqrt{2}\,E_{1113} & \sqrt{2}\,E_{1112} \\ E_{1122} & E_{2222} & E_{2233} & \sqrt{2}\,E_{2223} & \sqrt{2}\,E_{1223} & \sqrt{2}\,E_{1222} \\ E_{1133} & E_{2233} & E_{3333} & \sqrt{2}\,E_{2333} & \sqrt{2}\,E_{1333} & \sqrt{2}\,E_{1233} \\ \sqrt{2}\,E_{1123} & \sqrt{2}\,E_{2223} & \sqrt{2}\,E_{2333} & 2E_{2323} & 2E_{2331} & 2E_{2312} \\ \sqrt{2}\,E_{1113} & \sqrt{2}\,E_{1223} & \sqrt{2}\,E_{1333} & 2E_{2331} & 2E_{1313} & 2E_{3112} \\ \sqrt{2}\,E_{1112} & \sqrt{2}\,E_{1222} & \sqrt{2}\,E_{1233} & 2E_{2312} & 2E_{3112} & 2E_{1212} \end{pmatrix}. \tag{4.3}$$

This matrix is called the Kelvin matrix and it is used, usually, for computations since it is the matrix representation of the elasticity tensor in an orthonormal basis (for instance, the matrix $\{\mathbf{E}^{-1}\}$ is simply equal to $\{\mathbf{E}\}^{-1}$). On the other side, if one simply aims at viewing the elasticity parameters, another notation can be used for the matrix of the elasticity tensor, called the Voigt matrix

$$[\mathbf{E}] = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & E_{1123} & E_{1113} & E_{1112} \\ E_{1122} & E_{2222} & E_{2233} & E_{2223} & E_{1223} & E_{1222} \\ E_{1133} & E_{2233} & E_{3333} & E_{2333} & E_{1333} & E_{1233} \\ E_{1123} & E_{2223} & E_{2333} & E_{2323} & E_{2331} & E_{2312} \\ E_{1113} & E_{1223} & E_{1333} & E_{2331} & E_{1313} & E_{3112} \\ E_{1112} & E_{1222} & E_{1233} & E_{2312} & E_{3112} & E_{1212} \end{pmatrix}. \tag{4.4}$$

4.2.2 Isotropy classes for $\mathrm{SO}(3)$-representation on $\mathbb{E}\mathrm{la}$

Consider the action of $\mathrm{SO}(3)$ on the vector space $\mathbb{E}\mathrm{la}$ of elasticity tensors given by (using Einstein notation)

$$(g \star \mathbf{E})_{ijk} = g_{ip} g_{jq} g_{kr} g_{ls} E_{pqrs}, \quad g \in \mathrm{SO}(3),\ \mathbf{E} \in \mathbb{E}\mathrm{la}.$$

The problem of classifying linear elastic materials according to their symmetries goes at least as far back as the work of Lord Kelvin ([107], [58]). From then, many researchers devoted a great effort to the problem especially in crystallographic theory since they took for granted that symmetries of elasticity tensors should be looked for within the set of crystal classes and they found seven groups of orthogonal tensors corresponding to seven crystal systems (for more details on crystallographic theory, one can refer to Backus [6], Rychlewski [97], Walpole [110], Cowin and Mehrabadi [24], Love [68], Federov [34] and many others). However, the requirements imposed by some symmetries that do not exist in crystal lattices could not be avoided which made the researchers in the domain settle for 10 symmetry classes for the elasticity tensors ([45],[24], [103], [112]) until 1996 when Forte-Vianello ([37]) proved that there exist exactly eight symmetry classes. Inspired by the observation of Khatkevich ([59]), Forte-Vianello clarified the mathematical problem about the symmetry classes of an elasticity tensor and removed the

link with crystallographic point groups which was extremely confusing and lead to the false assumption that there were ten, rather than eight. Later, Chadwick and coauthors confirmed the eight classes in ([17]).

Theorem 4.2.1. *(Forte-Vianello 1996 [37]) There exists 8 isotropy classes for the* SO(3)*-representation on the space of elasticity tensors* $\mathbb{E}\mathrm{la}$*, given by*

$$\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{D}_3], [\mathbb{D}_4], [\mathbb{O}], [\mathrm{O}(2)], [\mathrm{SO}(3)]\}\,.$$

The eight elasticity isotropy classes for the SO(3)-representation on $\mathbb{E}\mathrm{la}$ are depicted in Figure 4.1 with the mechanical nomenclature and arrows corresponding to the partial order $\preceq$ (an arrow from $[H_1]$ to $[H_2]$ means that $[H_1] \preceq [H_2]$, see subsection 1.2.2).

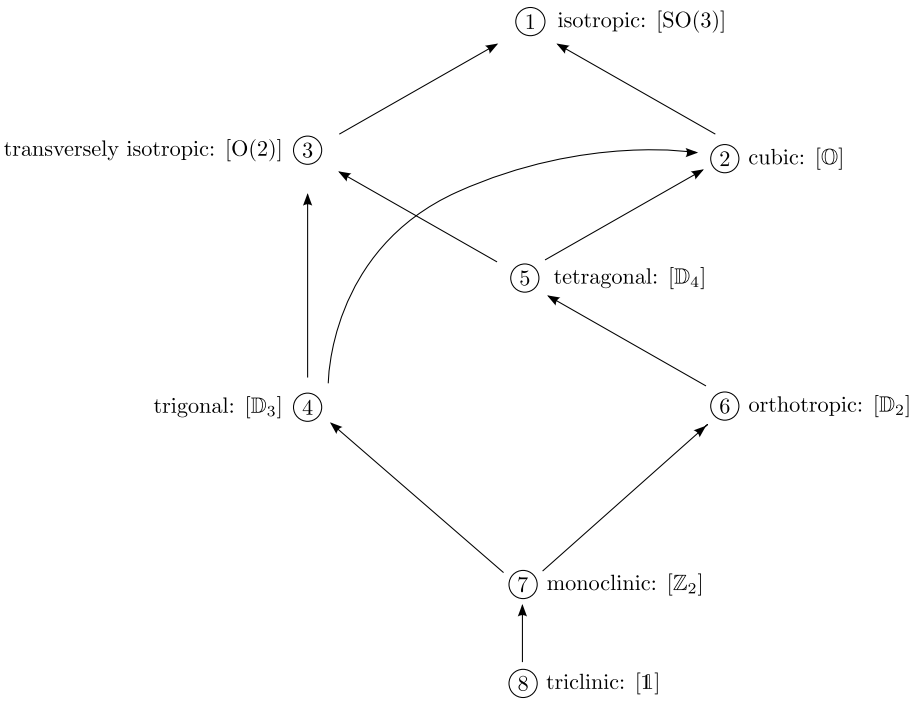

Figure 4.1: The poset of symmetry classes for $\mathbb{E}\mathrm{la}$ [53, 37].

4.2.3 Harmonic decomposition of the space of elasticity tensors

The vector space $\mathbb{E}\mathrm{la}$ can be decomposed into a direct sum of irreducible spaces (see section 3.2). Backus in [6] was the first to give such a decomposition to $\mathbb{E}\mathrm{la}$:

$$\mathbb{E}\mathrm{la} = \mathbb{H}^0(\mathbb{R}^3) \oplus \mathbb{H}^0(\mathbb{R}^3) \oplus \mathbb{H}^2(\mathbb{R}^3) \oplus \mathbb{H}^2(\mathbb{R}^3) \oplus \mathbb{H}^4(\mathbb{R}^3)$$

where $\mathbb{H}^n(\mathbb{R}^3)$, for $n = 0, 2, 4$, is the space of harmonic tensors of order n. Meaning that any $\mathbf{E} \in \mathbb{E}\mathrm{la}$ can be written as

$$\mathbf{E} = (\alpha, \beta, \mathbf{d}', \mathbf{v}', \mathbf{H}),$$

with $\alpha, \beta \in \mathbb{H}^0(\mathbb{R}^3)$ (called the *isotropic components* of $\mathbf{E}$), $\mathbf{d}', \mathbf{v}' \in \mathbb{H}^2(\mathbb{R}^3)$ (the *second-order harmonic components* of $\mathbf{E}$) and $\mathbf{H} \in \mathbb{H}^4(\mathbb{R}^3)$ (the *fourth-order harmonic component* of $\mathbf{E}$). The

harmonic components α, β, $\mathbf{d}'$ and $\mathbf{v}'$ are given by

$$\alpha = \mathrm{tr}(\mathbf{d}), \qquad \beta = \mathrm{tr}(\mathbf{v}), \qquad \mathbf{d}' := \mathbf{d} - \frac{1}{3}\,\mathrm{tr}(\mathbf{d})\,\mathbf{q}, \qquad \mathbf{v}' := \mathbf{v} - \frac{1}{3}\,\mathrm{tr}(\mathbf{v})\,\mathbf{q}.$$

where $\mathbf{d} := \mathrm{tr}_{12}\,\mathbf{E}$ ($d_{ij} = E_{kkij}$, using Einstein notation) and $\mathbf{v} := \mathrm{tr}_{13}\,\mathbf{E}$ ($v_{ij} = E_{kikj}$). In other words, an elasticity tensor $\mathbf{E} \in \mathbb{E}\mathrm{la}$ admits the following explicit harmonic decomposition [6]:

$$\mathbf{E} = \mathbf{E}^{iso} + \mathbf{q} \underset{(4)}{\otimes} \mathbf{a} + \mathbf{q} \underset{(2,2)}{\otimes} \mathbf{b} + \mathbf{H}. \tag{4.5}$$

where

$$\mathbf{E}^{iso} = \frac{1}{15}\,(\alpha + 2\beta)\,\mathbf{q} \underset{(4)}{\otimes} \mathbf{q} + \frac{1}{6}\,(\alpha - \beta)\,\mathbf{q} \underset{(2,2)}{\otimes} \mathbf{q}, \tag{4.6}$$

$$\alpha = \mathrm{tr}(\mathbf{d}), \qquad \beta = \mathrm{tr}(\mathbf{v}), \tag{4.7}$$

and

$$\mathbf{a} = \frac{2}{7}(\mathbf{d}' + 2\mathbf{v}'), \qquad \mathbf{b} = 2(\mathbf{d}' - \mathbf{v}'). \tag{4.8}$$

with $\mathbf{d}'$ and $\mathbf{v}'$ defined by (4.2.3).

In (4.5), $\mathbf{q}$ is the Euclidean canonical bilinear 2-form represented by the components $(\delta_{ij})_{i,j\in\{1,2,3\}}$ in any orthonormal basis and the tensor products $\underset{(4)}{\otimes}$ and $\underset{(2,2)}{\otimes}$, between symmetric second-order tensors $\mathbf{a}$, $\mathbf{b}$, are defined as follows (using Einstein notation):

$$(\mathbf{a} \underset{(4)}{\otimes} \mathbf{b})_{ijkl} = \frac{1}{6}(a_{ij}b_{kl} + b_{ij}a_{kl} + a_{ik}b_{jl} + b_{ik}a_{jl} + a_{il}b_{jk} + b_{il}a_{jk}),$$

and

$$(\mathbf{a} \underset{(2,2)}{\otimes} \mathbf{b})_{ijkl} = \frac{1}{6}(2a_{ij}b_{kl} + 2b_{ij}a_{kl} - a_{ik}b_{jl} - a_{il}b_{jk} - b_{ik}a_{jl} - b_{il}a_{jk}).$$

4.3 O(3)-representation on the space of piezoelectricity tensors

To describe the electric state of a material, we use the piezoelectricity law. In fact, an electric displacement is induced in response to an applied mechanical stress and this property is modeled by a third order tensor $\mathbf{P}$, called *piezoelectricity tensor*. The constitutive equation for this law is given by

$$\boldsymbol{d} = \mathbf{P} : \boldsymbol{\sigma} \quad (d_i = P_{ijk}\sigma_{jk},\ i,j,k \in \{1,2,3\})$$

where $\boldsymbol{d}$ is the electric displacement vector and $\boldsymbol{\sigma}$ is the stress tensor.

4.3.1 The piezoelectricity tensor

The *piezoelectricity* tensor is a third order tensor

$$\mathbf{P} : \mathbb{S}^2(\mathbb{R}^3) \to \mathbb{R}^3$$

with indicial symmetry $P_{ijk} = P_{ikj}$, $i,j,k \in \{1,2,3\}$ ([33]). We denote by $\mathbb{P}\mathrm{iez}$ the space of piezoelectricity tensors.

A piezoelectricity tensor has 18 independent components and can be represented by a 3×6 matrix, either in so-called Voigt notation (to view the piezoelectricity parameters)

$$[\mathbf{P}] = \begin{pmatrix} P_{111} & P_{122} & P_{133} & P_{123} & P_{113} & P_{112} \\ P_{211} & P_{222} & P_{233} & P_{223} & P_{213} & P_{212} \\ P_{311} & P_{322} & P_{333} & P_{323} & P_{313} & P_{312} \end{pmatrix} \tag{4.9}$$

or in so-called Kelvin notation (useful for computations since it is the matrix representation of the tensor in an orthonormal basis)

$$\{\mathbf{P}\} = \begin{pmatrix} P_{111} & P_{122} & P_{133} & \sqrt{2}P_{123} & \sqrt{2}P_{113} & \sqrt{2}P_{112} \\ P_{211} & P_{222} & P_{233} & \sqrt{2}P_{223} & \sqrt{2}P_{213} & \sqrt{2}P_{212} \\ P_{311} & P_{322} & P_{333} & \sqrt{2}P_{323} & \sqrt{2}P_{313} & \sqrt{2}P_{312} \end{pmatrix}. \tag{4.10}$$

4.3.2 Isotropy classes for $\mathrm{O}(3)$-representation on $\mathbb{P}\mathrm{iez}$

Consider the action of $\mathrm{O}(3)$ on the vector space $\mathbb{P}\mathrm{iez}$ of piezoelectricity tensors given by

$$(g \star \mathbf{P})_{ijk} = g_{ip} g_{jq} g_{kr} P_{pqr}, \quad g \in \mathrm{O}(3),\ \mathbf{P} \in \mathbb{P}\mathrm{iez}.$$

Obviously, the physical nature of the piezoelectric material is not affected by this transformation, only its constitutive tensors are transformed. The possible anisotropies of a constitutive law are modeled on the symmetry classes of the associated representation. Symmetry classes of the piezoelectricity tensors can be found in many works such as [84, 113, 111, 82, 114] who followed the approach of Forte–Vianello [37] in the case of the elasticity tensor. Later, Olive et al. proposed a general algorithm in [87, 88, 86, 89] to simplify the determination of symmetry classes based on the definition of clips operations on conjugacy classes (a strategy initiated by Chossat et al. [19, 18] and defined in subsection 3.3.2) and the harmonic decomposition defined in subsection 4.3.3. By these means, the 16 symmetry classes of $\mathbb{P}\mathrm{iez}$ are directly obtained in the following theorem (the notations and definitions of $\mathrm{O}(3)$-subgroups are fully given in section 3.1):

Theorem 4.3.1 (Olive et al. 2021 [89]). *A conjugacy class of a closed subgroup of* $\mathrm{O}(3)$ *is a symmetry class of a tensor* $\mathbf{P} \in \mathbb{P}\mathrm{iez}$ *if and only if it belongs to the 16 elements set of symmetry classes:*

$$\left\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{Z}_2^-], [\mathbb{Z}_4^-], [\mathbb{D}_2], [\mathbb{D}_3], [\mathbb{D}_4^d], [\mathbb{D}_6^d], [\mathrm{SO}(2)], [\mathrm{O}(2)], [\mathrm{O}(2)^-], [\mathbb{O}^-], [\mathrm{O}(3)]\right\}.$$

4.3.3 Harmonic decomposition of the space of piezoelectricity tensors

The harmonic decomposition of the space $\mathbb{P}\mathrm{iez}$ for the $\mathrm{O}(3)$-representation is given by

$$\mathbb{P}\mathrm{iez} \simeq \mathbb{H}^3 \oplus \mathbb{H}^{\#2} \oplus \mathbb{H}^1 \oplus \mathbb{H}^1,$$

where, if $n \in \mathbb{N}$, $\mathbb{H}^n$ denotes the space of nth-order harmonic tensors endowed with the standard representation and $\mathbb{H}^{\#n}$ refers to the same space endowed with the twisted representation (3.2) (see also [89]).

Any piezoelectricity tensor $\mathbf{P} \in \mathbb{P}\mathrm{iez}$ can be written as

$$\mathbf{P} = (\boldsymbol{v}, \boldsymbol{w}, \mathbf{a}, \mathbf{h})$$

with $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{H}^1(\mathbb{R}^3)$, $\mathbf{a} \in \mathbb{H}^{\#2}(\mathbb{R}^3)$ and $\mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$.

Let $\odot$ be the symmetric tensor product and $\mathbf{P}^s \in \mathbb{S}^3(\mathbb{R}^3)$ denote the totally symmetric part of $\mathbf{P}$ (of components $(\mathbf{P}^s)_{ijk} = \frac{1}{3}(P_{ijk} + P_{jik} + P_{kji})$). Any piezoelectricity tensor $\mathbf{P} \in \mathbb{P}\mathrm{iez}$ can be decomposed as the sum

$$\mathbf{P} = \mathbf{g} + \mathbf{h}$$

where

$$\mathbf{h} := \mathbf{P}^s - \frac{3}{5}\mathbf{q} \odot \mathrm{tr}(\mathbf{P}^s) \in \mathbb{H}^3(\mathbb{R}^3), \tag{4.11}$$

is the *leading harmonic part* of $\mathbf{P}$, and

$$\mathbf{g} := \mathbf{P} - \mathbf{h} = (\boldsymbol{v}, \boldsymbol{w}, \mathbf{a}),$$

is orthogonal to $\mathbf{h}$ (*i.e.* $\langle \mathbf{g}, \mathbf{h} \rangle = g_{ijk}h_{ijk} = 0$).

Remark 4.3.2. *The third-order tensors* $\mathbf{g} = \mathbf{g}(\mathbf{P})$ *and* $\mathbf{h} = \mathbf{h}(\mathbf{P})$ *are linear covariants of* $\mathbf{P}$.

4.3.4 Characterization of the cubic class

Here we give the characterization of the cubic class $\Sigma_{[\mathbb{O}^-]}$ for piezoelectricity tensors.

Theorem 4.3.3. *Let* $\mathbf{P} = \mathbf{g} + \mathbf{h} \in \mathbb{P}\mathrm{iez}$ *be a piezoelectricity tensor, with* $\mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$ *its leading harmonic part, let*

$$\mathbf{d}_2 = \mathbf{h} : \mathbf{h} \qquad (\text{i.e., } (\mathbf{d}_2)_{ij} = h_{ikl}h_{klj}),$$

and $\mathbf{d}_2' = \mathbf{d}_2 - \frac{1}{3}\,\mathrm{tr}(\mathbf{d}_2)\,\mathbf{q}$ *be second-order covariants of* $\mathbf{P}$. *Then* $\mathbf{P} \in \overline{\Sigma}_{[\mathbb{O}^-]}$ *(is at least cubic) if and only if*

$$\mathbf{g} = 0 \quad \textit{and} \quad \mathbf{d}_2' = 0,$$

and $\mathbf{P} \in \Sigma_{[\mathbb{O}^-]}$ *(is cubic) if and only if furthermore* $\mathbf{h} \neq 0$.

The proof of this theorem is fully detailed in the appendix C of chapter 5 of this manuscript.

4.4 Isotropy classes for the coupled piezoelectricity law using clips operation between O(3)-subgroups

In the following, we denote by $\mathcal{J}(V)$ the set of isotropy classes of the representation of either SO(3) or O(3) on the vector space V.

As a consequence of lemma 3.3.2, the isotropy classes $\mathcal{J}(\mathcal{P}\mathrm{iez})$ can be deduced from isotropy classes $\mathbb{E}\mathrm{la}$, $\mathbb{P}\mathrm{iez}$ and $\mathbb{S}$:

$$\mathcal{J}(\mathcal{P}\mathrm{iez}) = (\mathcal{J}(\mathbb{E}\mathrm{la}) \circledcirc \mathcal{J}(\mathbb{P}\mathrm{iez})) \circledcirc \mathcal{J}(\mathbb{S}).$$

Recall from theorem 4.3.1 the isotropy classes of $\mathbb{P}\mathrm{iez}$ (the notations and definitions of O(3)-subgroups have been recalled in section 3.1):

$$\mathcal{J}(\mathbb{P}\mathrm{iez}) = \Big\{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{Z}_2^-], [\mathbb{Z}_4^-], [\mathbb{D}_2], [\mathbb{D}_3], [\mathbb{D}_4^d], [\mathbb{D}_6^d], \\ [\mathrm{SO}(2)], [\mathrm{O}(2)], [\mathrm{O}(2)^-], [\mathbb{O}^-], [\mathrm{O}(3)]\Big\}.$$

The symmetry classes for O(3)-representation on $\mathbb{E}\mathrm{la}$ and $\mathbb{S}$ are the same as the symmetry classes for SO(3)-representation which can be found in [38] and [91], except that each type I subgroup occurring in the list of isotropy classes has to be replaced by the corresponding type II subgroup (see section 3.1). Indeed, $-\mathrm{I}$ acts trivially on $\mathbb{E}\mathrm{la}$ and $\mathbb{S}$. Hence, the isotropy classes for the O(3)-representation on $\mathbb{E}\mathrm{la}$ and $\mathbb{S}$ are given by

$$\mathcal{J}(\mathbb{E}\mathrm{la}) = \{[\mathbb{1}], [\mathbb{Z}_2 \oplus \mathbb{Z}_2^c], [\mathbb{D}_2 \oplus \mathbb{Z}_2^c], [\mathbb{D}_3 \oplus \mathbb{Z}_2^c], [\mathbb{D}_4 \oplus \mathbb{Z}_2^c], [\mathbb{O} \oplus \mathbb{Z}_2^c], [\mathrm{O}(2) \oplus \mathbb{Z}_2^c], [\mathrm{SO}(3) \oplus \mathbb{Z}_2^c]\},$$

and

$$\mathcal{J}(\mathbb{S}) = \{[\mathbb{D}_2 \oplus \mathbb{Z}_2^c], [\mathrm{O}(2) \oplus \mathbb{Z}_2^c], [\mathrm{SO}(3) \oplus \mathbb{Z}_2^c]\}.$$

We deduce the isotropy classes of the Piezoelectricity coupled law $\mathcal{P}\mathrm{iez} = \mathbb{E}\mathrm{la} \oplus \mathbb{P}\mathrm{iez} \oplus \mathbb{S}$ from lemma 3.3.2 by calculating the clips operations between the isotropy classes of $\mathbb{E}\mathrm{la}$, $\mathbb{P}\mathrm{iez}$ and $\mathbb{S}$ (see Table 3.2 and Table 3.3 for clips between type II and III O(3)-subgroups and [86, table 1] for clips between two type I and remark 3.1 (1) for type I with type II and two type II).

Theorem 4.4.1. *[5] There exist 25 isotropy classes for the Piezoelectricity coupled law* $\mathbb{E}\mathrm{la} \oplus \mathbb{P}\mathrm{iez} \oplus \mathbb{S}$ *given by*

$$\mathcal{J}(\mathcal{P}iez) = \{[\mathbb{1}], [\mathbb{Z}_2], [\mathbb{Z}_3], [\mathbb{Z}_4], [\mathbb{D}_2], [\mathbb{D}_3], [\mathbb{D}_4], [\mathrm{SO}(2)], [\mathrm{O}(2)], [\mathrm{O}(3)], \\ [\mathbb{Z}_2 \oplus \mathbb{Z}_2^c], [\mathbb{D}_2 \oplus \mathbb{Z}_2^c], [\mathbb{D}_3 \oplus \mathbb{Z}_2^c], [\mathbb{D}_4 \oplus \mathbb{Z}_2^c], [\mathbb{O} \oplus \mathbb{Z}_2^c], [\mathrm{O}(2) \oplus \mathbb{Z}_2^c], \\ [\mathbb{Z}_2^-], [\mathbb{Z}_4^-], [\mathbb{D}_2^z], [\mathbb{D}_3^z], [\mathbb{D}_4^z], [\mathbb{D}_2^d], [\mathbb{D}_4^d], [\mathbb{D}_6^d], [\mathbb{O}^-], [\mathrm{O}(2)^-]\Big\}.$$

Chapter 5

Distance to isotropy strata by Lasserre polynomial optimization method

This chapter is an ArXiv preprint [3] in which we solve the problem of the distance to isotropy strata using Lasserre's method for polynomial optimization problems. We take advantage of the characterization of the isotropy strata by polynomial equations in some cases (elasticity and piezoelectricity for instance) to formulate the problem of determining the closest tensor belonging to a specific isotropy stratum to an experimental one into a polynomial optimization problem. In other words, from a mechanical problem, we construct a minimization problem of a polynomial function under polynomial constraints. Lasserre provides a method for solving such problems that consists on building a hierarchy of relaxed semidefinite problems converging to the optimal minimum under some conditions. With this method, we were able to solve the problem for some numerical examples in cubic elasticity and cubic piezoelectricity for instance. Despite its efficiency in converging to the desired solution in a small amount of time with high numerical precision, this method is not always convenient. In fact, when the number of variables and the number of constraints increase, converging to the optimal solution becomes more difficult.

DISTANCE TO A CONSTITUTIVE TENSOR ISOTROPY STRATUM BY LASSERRE POLYNOMIAL OPTIMIZATION METHOD

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Abstract. We give a detailed description of a polynomial optimization method allowing to solve a problem in continuum mechanics: the determination of the elasticity or the piezoelectricity tensor of a specific isotropy stratum the closest to a given experimental tensor, and the calculation of the distance to the given tensor from the considered isotropy stratum. We take advantage of the fact that the isotropy strata are semialgebraic sets to show that the method, developed by Lasserre and coworkers which consists in solving polynomial optimization problems with semialgebraic constraints, successfully applies.

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1. Introduction

In mechanics, *linear constitutive laws* are described by the orbit space of a representation of the three-dimensional orthogonal group on the vector space of the considered *constitutive tensors* $\mathbf{T}$ [45, 13, 21]. This orbit space is endowed with a natural stratification by *isotropy classes* $[H]$, the strata $\Sigma_{[H]}$ being the set of tensors with symmetry group conjugate to H.

The symmetry group of a measured (raw) tensor $\mathbf{T}_0$ is in general trivial. However, in practice, appealing to Curie principle—*the symmetries of the causes are to be found in the effects*—a symmetry of a constitutive tensor is often expected by observing the micro-structure of a material [5, 24, 25]. For instance, the elasticity tensor of a single crystal alloy with cubic crystal network is expected to be cubic ($[\mathbb{O}]$, see figure 1), the piezoelectric tensor of an aluminum nitride (AlN) alloyed with rocksalt transition metal nitrides is expected to become cubic ($[\mathbb{O}^-]$) for a high chromium concentration [49]. The mechanical problem thus comes down to the

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computation of the distance $d(\mathbf{T}_0, \overline{\Sigma}_{[H]})$ of a raw constitutive tensor $\mathbf{T}_0$ to a closed isotropy stratum $\overline{\Sigma}_{[H]}$.

In linear elasticity, which involves a fourth-order tensor $\mathbf{E}$, the distance to an isotropy stratum has been formulated as the minimization problem [27, 25, 18, 54, 12]

$$\min_{\mathbf{E}\in\overline{\Sigma}_{[H]}} \|\mathbf{E}_0 - \mathbf{E}\|, \qquad \mathbf{E} = \rho_4(g)\mathbf{A}, \qquad \mathbf{A} \in \mathbb{F}\mathrm{ix}(H),\ g \in \mathrm{SO}(3),$$

with the natural parameterization by *normal form* $\mathbf{A}$ (a fixed point set for a representative symmetry group H) and *rotation* g. This problem has, however, many local minima and several global minima, making the determination of all the solutions numerically difficult.

In this paper, we formulate the computation of the distance to an isotropy stratum as a polynomial optimization problem. To do so, we make use of the property that the closed isotropy strata $\overline{\Sigma}_{[H]}$ are basic closed semialgebraic sets [1, 2, 63, 65]. For the fourth-order elasticity tensor, an explicit characterization of the closed strata $\overline{\Sigma}_{[H]}$ by polynomial equations and inequalities has recently been obtained, by means of polynomial covariants [61, Theorem 10.2]. Since such a result is not yet available in piezoelectricity, we have provided in theorem 7.2 a polynomial characterization of the cubic symmetry stratum $\overline{\Sigma}_{[\mathbb{O}^-]}$ for the third-order piezoelectricity tensor.

We formulate the distance problems in question in such a way that we can apply a semialgebraic optimization method designed by Lasserre and coworkers [40, 41, 42, 33, 37] to compute directly the global miminum of a polynomial function over polynomial constraints describing a basic closed semialgebraic set. This method consists in building a sequence of semidefinite programs whose optimal values converge to the desired minimum, under some hypothesis on the constraints. The benefit is that there exist efficient algorithms to solve numerically semidefinite programs, based on methods used in linear programming [17, 47, 73], such as the ellipsoid method [30] or the interior point method [56, 3, 57, 71, 36, 8, 9, 19]. The considered algorithm has been implemented by Lasserre and Henrion [33] in a Matlab freeware, named GloptiPoly [32], that aims to solve a sequence of relaxed semidefinite programs using SeDuMi (a Matlab toolbox for solving semidefinite programs created by Sturm [69, 70]). Moreover, this algorithm, when its stopping criterion is satisfied, extracts (approximated) minimizers for the considered minimized function.

Organization of the paper. The paper is organized as follows. In section 2, we recall basic material on isotropy classes and we pose the problem of the distance to an isotropy class. In section 3, we introduce polynomial optimization and its formulation to semidefinite programs. In section 3 and section 4, we describe the Lasserre and coworkers method for solving polynomial optimization problems with semialgebraic constraints as well as the corresponding algorithm, implemented as the software GloptiPoly. As a direct application, we deal with three examples of constitutive tensors. In section 5, we illustrate the method with the academic example of the distance of a symmetric second-order tensor to the transversely isotropic stratum $\overline{\Sigma}_{[\mathrm{O}(2)]}$. In section 6, we compute the distance of an experimental elasticity (fourth-order) tensor of a Nickel-based single crystal superalloy to the cubic stratum $\overline{\Sigma}_{[\mathbb{O}]}$, and consequently we extract the cubic elasticity tensor the closest to the experimental one. Finally, in section 7, we detail how polynomial optimization allows to find the cubic piezoelectricity (third-order) tensors, in $\overline{\Sigma}_{[\mathbb{O}^-]}$, the closest to raw tensors for wurtzite alloys.

All the tensorial components will be expressed with respect to an orthonormal basis. Hence, no distinction will be made between covariant and contravariant components. The notation $\mathbf{q} = (\delta_{ij})$ stands for the Euclidean metric tensor.

2. Isotropy classes and strata – Distance to an isotropy stratum

Let G be a compact group and $\rho : G \to \mathrm{GL}(\mathbb{V})$ be a continuous representation of G on a finite dimensional real vector space $\mathbb{V}$. Given $\boldsymbol{v} \in \mathbb{V}$, its *orbit* is the subset of $\mathbb{V}$ defined by

$$\mathrm{Orb}(\boldsymbol{v}) := \{\rho(g)\boldsymbol{v};\ g \in G\},$$

and its *symmetry group* (or isotropy group) is defined as

$$G_{\boldsymbol{v}} := \{g \in G;\ \rho(g)\boldsymbol{v} = \boldsymbol{v}\}\,.$$

The concept of symmetry group allows to define an equivalence relation on $\mathbb{V}$, which is *coarser* than the relation "to be in the same orbit" and defined as follows: two vectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ *have the same isotropy class* (or same symmetry class in mechanics [22, 23]) if they have conjugate symmetry groups. In the following, we shall denote by

$$[H] := \left\{gHg^{-1};\ g \in G\right\}$$

the conjugacy class of the subgroup H of G. To each conjugacy class $[H]$, where H is a closed subgroup of G, corresponds the subset of $\mathbb{V}$ defined by

$$\Sigma_{[H]} := \{\boldsymbol{v} \in \mathbb{V};\ [G_{\boldsymbol{v}}] = [H]\}\,.$$

If this subset is not empty, $[H]$ is called an *isotropy class* and $\Sigma_{[H]}$ is the *isotropy stratum associated to* $[H]$. It is known (see [55, 10, 48]) that there is only a finite number of isotropy classes for any finite dimensional representation of a compact group.

The set of conjugacy classes $[H]$ of closed subgroups of a compact group is endowed with a partial order relation (reflexivity and transitivity are direct and true even if G is not compact but anti-symmetry requires the compacity of G [11, Proposition 1.9]), given by

$$[H] \preceq [K] \iff \exists g \in G, \quad gHg^{-1} \subset K.$$

Due to the order relation defined on the conjugacy classes, we define a *closed stratum* to be the set consisting of vectors having *at least the symmetry* $[H]$*, denoted by* $\overline{\Sigma}_{[H]}$*, and defined by*

$$\overline{\Sigma}_{[H]} = \{\boldsymbol{v} \in \mathbb{V};\ [H] \preceq [G_{\boldsymbol{v}}]\} = \bigcup_{[H]\preceq[K]} \Sigma_{[K]}.$$

The isotropy stratum $\Sigma_{[H]}$ and the closed isotropy stratum $\overline{\Sigma}_{[H]}$ are semialgebraic sets [1, 2, 63, 65], *i.e* defined by polynomial equations and inequalities [14, 9]. Actually, if G is a subgroup of $\mathrm{GL}(\mathbb{V})$, we can give a direct proof of this fact. Indeed, if G is a compact subgroup of $\mathrm{GL}(\mathbb{V})$, G is a real algebraic set by [62, Chapter 3, paragraph 4, Theorem 5]. Notice that so is the subset $G_{\boldsymbol{v}}$, if $\boldsymbol{v} \in \mathbb{V}$, as it is described by polynomial equations in the coefficients of the matrices of the real algebraic set G. Now, since H is a closed subgroup of G, H is in particular a compact subgroup of $\mathrm{GL}(\mathbb{V})$ and then a real algebraic set as well. As a consequence, the closed isotropy stratum

$$\overline{\Sigma}_{[H]} = \left\{\boldsymbol{v} \in \mathbb{V};\ \exists g \in G, \forall h \in H, ghg^{-1}\boldsymbol{v} = \boldsymbol{v}\right\},$$

and the isotropy stratum

$$\Sigma_{[H]} = \left\{\boldsymbol{v} \in \mathbb{V};\ \exists g \in G, \forall h \in H, ghg^{-1}\boldsymbol{v} = \boldsymbol{v} \ \text{ and } \ \exists g' \in G, \forall k \in G, k\boldsymbol{v} = \boldsymbol{v} \Rightarrow g'kg'^{-1} \in H\right\},$$

are both described by *first-order formulae* (in the sense of [9, Definition 2.2.3]) so that the sets $\overline{\Sigma}_{[H]}$ and $\Sigma_{[H]}$ are semialgebraic sets by [9, Proposition 2.2.4] (the latter cited result is an avatar of *Tarski-Seidenberg theorem* which is an angular stone of semialgebraic geometry).

We shall introduce the distance of a vector $\boldsymbol{v}_0 \in \mathbb{V}$ to the closed isotropy stratum $\overline{\Sigma}_{[H]}$

$$\Delta(\boldsymbol{v}_0, \overline{\Sigma}_{[H]})^2 := \min_{\boldsymbol{v}\in\overline{\Sigma}_{[H]}} \|\boldsymbol{v}_0 - \boldsymbol{v}\|^2, \tag{1}$$

for some G-invariant norm $\|\cdot\|$. A minimizer will be denoted by $\boldsymbol{v}^*$.

Examples of interest for the present work are provided by Continuum Mechanics, for which G is either $\mathrm{SO}(3)$ or $\mathrm{O}(3)$, $\mathbb{V}$ is a space of tensors on $\mathbb{R}^3$, endowed with the invariant norm

$$\|\mathbf{T}\| := \sqrt{T_{i_1\dots i_n}T_{i_1\dots i_n}},$$

and the action on a tensor $\mathbf{T}$ is written (in an orthonormal basis)

$$(\rho(g)\mathbf{T})_{i_1\dots i_n} := g_{i_1}{}^{j_1}\dots g_{i_n}{}^{j_n}T_{j_1\dots j_n}, \quad \mathbf{T} \in \mathbb{V},\ g \in G.$$

Finally, the $\mathrm{O}(3)$-subgroups will be denoted according to the notations in [29].

Example 2.1. In elasticity,

$$\mathbb{V} = \mathbb{E}\mathrm{la} = \mathbb{S}^2(\mathbb{S}^2(\mathbb{R}^3)) = \left\{\mathbf{E} \in \otimes^4\mathbb{R}^3,\, E_{ijkl} = E_{jikl} = E_{klij}\right\}$$

is the 21-dimensional vector space of elasticity tensors, and $G = \mathrm{SO}(3)$. In that case there are exactly eight isotropy classes $[\mathbb{1}]$, $[\mathbb{Z}_2]$, $[\mathbb{D}_2]$, $[\mathbb{D}_3]$, $[\mathbb{D}_4]$, $[\mathrm{O}(2)]$, $[\mathbb{O}]$, $[\mathrm{SO}(3)]$ [22], and the problem of the distance to an elasticity isotropy stratum has been investigated in [74, 25, 18, 54, 38, 39].

Example 2.2. In piezoelectricity,

$$\mathbb{V} = \mathbb{P}\mathrm{iez} = \left\{\mathbf{e} \in \otimes^3\mathbb{R}^3,\, \mathrm{e}_{ijk} = \mathrm{e}_{ikj}\right\}$$

is the 18-dimensional vector space of piezoelectricity tensors, and $G = \mathrm{O}(3)$. In that case there are exactly 16 isotropy classes $[\mathbb{1}]$, $[\mathbb{Z}_2]$, $[\mathbb{Z}_3]$, $[\mathbb{D}_2^z]$, $[\mathbb{D}_3^z]$, $[\mathbb{Z}_2^-]$, $[\mathbb{Z}_4^-]$, $[\mathbb{D}_2]$, $[\mathbb{D}_3]$, $[\mathbb{D}_4^d]$, $[\mathbb{D}_6^d]$, $[\mathrm{SO}(2)]$, $[\mathrm{O}(2)]$, $[\mathrm{O}(2)^-]$, $[\mathbb{O}^-]$, $[\mathrm{O}(3)]$ [58, 76, 60], and the problem of the distance to a piezoelectricity isotropy stratum has been investigated in [77].

When polynomial equations and/or inequalities characterizing the semialgebraic set $\overline{\Sigma}_{[H]}$ are known (see [6, 61]), the distance to an isotropy stratum problem (1) reduces to minimize a polynomial function (the quadratic function $\Delta(\,\cdot\,,\overline{\Sigma}_{[H]})^2$) under polynomial constraints. In that case, we can solve the distance to an isotropy stratum problem using *polynomial and semialgebraic optimization* [42, 44, 53, 66], which allows to approximate numerically the global minimum of the function $\Delta(\,\cdot\,,\overline{\Sigma}_{[H]})^2$.

3. Semialgebraic optimization method

The problem of determining the constitutive tensor having a specific symmetry the closest to an experimental one can be viewed as an example of the problem of minimizing a polynomial function over polynomial constraints

$$f^* = \inf\left\{f(\boldsymbol{x});\ \boldsymbol{x} \in K\right\}, \tag{2}$$

where $f \in \mathbb{R}[X] := \mathbb{R}[X_1, \ldots, X_n]$, $\boldsymbol{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ and K is a basic closed semialgebraic set

$$K = \{\boldsymbol{x} \in \mathbb{R}^n;\ g_1(\boldsymbol{x}) \geq 0, \ldots, g_m(\boldsymbol{x}) \geq 0\},$$

with $g_1, \ldots, g_m \in \mathbb{R}[X]$ (see [14, 9] for self-contained references on semialgebraic geometry).

We now describe *Lasserre's method* [40, 42], that will allow us to solve numerically the problem of the distance from an experimental tensor to a closed stratum. The method consists in constructing a sequence of semidefinite programs whose optimal values form a nondecreasing sequence which converges to the optimum f^*.

In this section, apart from theorem 4.1 which is a refinement of [42, Theorem 6.2], there is no original statement: we give the essential steps and results of the approach for pedagogical reasons and to be self-contained. For more details on Lasserre's method and the involved mathematical results and background, we refer to [42, 44, 66].

The first step of the method is to notice that the optimization problem (2) can be reformulated as

$$f^* = \inf\left\{\int_{\mathbb{R}^n} f \mathrm{d}\mu;\ \mu \text{ probability measure on } \mathbb{R}^n \text{ with support in } K\right\}. \tag{3}$$

Indeed, for $\boldsymbol{x} \in K$, if $\delta_{\boldsymbol{x}}$ denotes the probability Dirac measure on $\mathbb{R}^n$ at $\boldsymbol{x}$, we have $f(\boldsymbol{x}) = \int f \mathrm{d}\delta_{\boldsymbol{x}}$ and, conversely, if μ is a probability measure on $\mathbb{R}^n$ with support in K,

$$\int_{\mathbb{R}^n} f(\boldsymbol{x})\mathrm{d}\mu(\boldsymbol{x}) \geq \int_{\mathbb{R}^n} f^* \mathrm{d}\mu(\boldsymbol{x}) = f^*.$$

Now, if $(y_\alpha)_{\alpha\in\mathbb{N}^n}$ is a sequence of real numbers, denote by $M(y)$ the infinite symmetric matrix

$$(y_{\alpha+\beta})_{\alpha,\beta\in\mathbb{N}^n},$$

(called the *moment matrix associated to* y) and, if $g = \sum_{\beta\in\mathbb{N}^n} g_\beta X^\beta$, set

$$g \cdot y := \left(\sum_{\beta\in\mathbb{N}^n} g_\beta y_{\alpha+\beta} \right)_{\alpha\in\mathbb{N}^n} \in \mathbb{R}^{\mathbb{N}^n}.$$

Under an hypothesis called the *Archimedean hypothesis*, we can write the optimization problem (3) as

$$f^* = \inf_{y\in\mathbb{R}^{\mathbb{N}^n}} \left\{ \langle f, y\rangle;\ y_{(0,\dots,0)} = 1,\ M\left(g_i \cdot y\right) \succeq 0,\ i = 0,\dots,m \right\} \tag{4}$$

where, if $y \in \mathbb{R}^{\mathbb{N}^n}$, $\langle f, y\rangle := \sum_\alpha f_\alpha y_\alpha$, and $g_0 := 1$. Here, if M is a finite or infinite matrix with real coefficients, $M \succeq 0$ means that M is positive semidefinite (an infinite symmetric matrix is called positive semidefinite if all its principal submatrices are positive semidefinite). The formulation (4) is a direct consequence of the following solution of the moment problem on K.

Theorem 3.1 (Putinar, Jacobi–Prestel)**.** *Suppose that the polynomials $g_1,\dots,g_m$ describing K satisfy the Archimedean hypothesis. Then, for all $y \in \mathbb{R}^{\mathbb{N}^n}$, y has a representative measure on K (i.e. there exists a finite Borel measure μ on $\mathbb{R}^n$ with support in K such that, for any $\alpha \in \mathbb{N}^n$, $y_\alpha = \int_{\mathbb{R}^n} \boldsymbol{x}^\alpha \mathrm{d}\mu(\boldsymbol{x})$) if and only if the moment matrices $M(y)$, $M(g_1\cdot y),\dots,M(g_m\cdot y)$ are positive semidefinite.*

This statement is a reformulation of [42, theorem 2.44] and is due to Putinar ([64]) and Jacobi–Prestel ([35]). We recall the proof below but, first, we have to define the essential *Archimedean hypothesis*.

Definition 3.2. Consider the $\mathbb{R}$-module

$$\mathbf{M}(g_1,\dots,g_m) := \left\{ \sigma_0 + \sum_{i=1}^m \sigma_i g_i;\ \sigma_0,\dots,\sigma_m \text{ sum of squares} \right\} \subset \mathbb{R}[X]$$

(a polynomial $p \in \mathbb{R}[X]$ is a *sum of squares* if there exist polynomials $p_1,\dots,p_N \in \mathbb{R}[X]$ such that $p = \sum_{j=1}^N p_j^2$). We say that the polynomials $g_1,\dots,g_m$ satisfy the *Archimedean hypothesis* (or that $\mathbf{M}(g_1,\dots,g_m)$ is an *Archimedean module*) if there exists a positive integer N such that

$$N - \sum_{i=1}^n X_i^2 \in \mathbf{M}(g_1,\dots,g_m).$$

We refer to [66, Theorem 1.1] (a result due to Schmüdgen) for a list of properties equivalent to the Archimedean hypothesis. Notice that if $g_1,\dots,g_m$ satisfy the Archimedean hypothesis, then

$$K = \{\boldsymbol{x} \in \mathbb{R}^n;\ g_1(\boldsymbol{x}) \geq 0,\dots,g_m(\boldsymbol{x}) \geq 0\}$$

is necessarily compact. The crucial point is that, if $g_1,\dots,g_m$ satisfy the Archimedean hypothesis, then we have access to Putinar's Positivstellensatz.

Theorem 3.3 (Putinar [64])**.** *Suppose that the polynomials $g_1,\dots,g_m$ describing K satisfy the Archimedean hypothesis, and let $p \in \mathbb{R}[X]$. If $p(K) \subset]0;+\infty[$, then $p \in \mathbf{M}(g_1,\dots,g_m)$.*

See also [66, section 2] and [44, section 3.7] for alternative proofs.

Proof of theorem 3.1. Let $y \in \mathbb{R}^{\mathbb{N}^n}$. The direct implication is actually true even if the polynomials $g_1,\dots,g_m$ do not satisfy the Archimedean hypothesis. Indeed, suppose that y has a representing measure μ on K. Now, take any vector $\mathbf{p} = (p_\alpha)_{\alpha\in\mathbb{N}^n}$ of $\mathbb{R}^{\mathbb{N}^n}$ with finitely many nonzero coordinates and set $p := \sum_\alpha p_\alpha X^\alpha$. If M is any matrix, denote by M^T its transpose. If g is any polynomial of $\{g_0,\dots,g_m\}$, we have then

$$\mathbf{p}^T M\left(g \cdot y\right) \mathbf{p} = \sum_{\alpha,\beta} p_\alpha p_\beta \left(\sum_\gamma g_\gamma \int_{\mathbb{R}^n} \boldsymbol{x}^{\alpha+\beta+\gamma} \mathrm{d}\mu(\boldsymbol{x}) \right) = \int_{\mathbb{R}^n} g(\boldsymbol{x}) p(\boldsymbol{x})^2 \mathrm{d}\mu(\boldsymbol{x}) \geq 0.$$

By definition, for all $\boldsymbol{x} \in K$, $g(\boldsymbol{x}) \geq 0$, and the support of μ is included in K.

Conversely, suppose that the matrices $M(y)$, $M(g_1 \cdot y), \ldots, M(g_m \cdot y)$ of y are positive semidefinite, and denote by L_y the linear mapping

$$p = \sum_\alpha p_\alpha X^\alpha \in \mathbb{R}[X] \mapsto \sum_\alpha p_\alpha y_\alpha \in \mathbb{R}.$$

Let $g \in \{g_0, \ldots, g_m\}$ and consider the symmetric bilinear form

$$\begin{array}{ccc} \mathbb{R}[X] \times \mathbb{R}[X] & \to & \mathbb{R} \\ (p,q) & \mapsto & L_y(pqg) \end{array},$$

which is represented by the localizing matrix $M(g \cdot y)$ in the canonical basis of $\mathbb{R}[X]$. In particular, for every polynomial p, if $\mathbf{p}$ denotes the vector $(p_\alpha)_{\alpha \in \mathbb{N}^n}$, we have

$$L_y\left(p^2 g\right) = \mathbf{p}^T M(g \cdot y)\, \mathbf{p} \geq 0$$

and, consequently, the linear mapping L_y has nonnegative values on $\mathbf{M}(g_1, \ldots, g_m)$. By Putinar's Positivstellensatz 3.3, this implies that L_y has nonnegative values on any polynomial $p \in \mathbb{R}[X]$ such that $p(K) \subset]0; +\infty[$.

If $p \in \mathbb{R}[X]$ satisfies $p(K) \subset [0; +\infty[$ then, for any positive real number ϵ, the polynomial $p + \epsilon$ has positive values on K so that $L_y(p) + \epsilon = L_y(p + \epsilon) \geq 0$, and therefore $L_y(p) \geq 0$. We can then apply Haviland's theorem ([31], see also [50, section 3.2] and Theorem 4.15 and section 4.6 of the up-to-date version of [44]) to the mapping L_y : there exists a measure μ on $\mathbb{R}^n$ with support in K such that $L_y(p) = \int_{\mathbb{R}^n} p(\boldsymbol{x}) \mathrm{d}\mu(\boldsymbol{x})$ for all $p \in \mathbb{R}[X]$. In particular, for all $\alpha \in \mathbb{N}^n$, we have

$$y_\alpha = L_y\left(X^\alpha\right) = \int_{\mathbb{R}^n} \boldsymbol{x}^\alpha \mathrm{d}\mu(\boldsymbol{x})$$

i.e., y is the moment sequence of the measure μ. □

From now on, we assume that the polynomials $g_1, \ldots, g_m$ satisfy the Archimedean hypothesis so that we can write

$$f^* = \inf_{y \in \mathbb{R}^{\mathbb{N}^n}} \left\{ \langle f, y \rangle;\ y_0 = 1,\ M(g_i \cdot y) \succeq 0,\ i = 0, \ldots, m \right\}, \tag{5}$$

where $y_0 := y_{(0,\ldots,0)}$.

Lasserre's method to solve the optimization problem (4) consists, then, in *relaxing* this infinite-dimensional problem into a sequence of finite-dimensional problems which are *semidefinite programs*. *Semidefinite programs*, or SDP's, are optimization problems over finite positive semidefinite symmetric matrices which generalize linear programs, and for which there exist efficient algorithms of numerical resolution. SDP-solving algorithms include methods inspired by the ones used in linear programming, such as interior point methods (see for instance the references [3, 72, 69, 71, 26, 75]).

Below, we follow Lasserre's notations in [42, section 6.1.1]. First, if $k \in \mathbb{N}$, let

$$\Lambda(k) := \{(\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n; \alpha_1 + \cdots + \alpha_n \leq k\}$$

and, if $y \in \mathbb{R}^{\Lambda(2k)}$ and $k' \in \mathbb{N}$ satisfies $k' \leq k$, set $M_{k'}(y) := (y_{\alpha+\beta})_{\alpha,\beta \in \Lambda(k')}$. If $g \in \mathbb{R}[X]$, set

$$g \cdot y := \left(\sum_{\beta \in \mathbb{N}^n} g_\beta y_{\alpha+\beta} \right)_{\alpha \in \Lambda(k)} \in \mathbb{R}^{\Lambda(k)}.$$

Finally, for $i \in \{0, \ldots, n\}$, denote $v_i := \left\lceil \frac{\deg(g_i)}{2} \right\rceil$ (notice that $v_0 = 0$) and let d_0 be the integer $\max\left(\left\lceil \frac{\deg(f)}{2} \right\rceil, v_1, \ldots, v_m \right)$.

For d any integer such that $d \geq d_0$, we then consider the optimization problem

$$\rho_d = \inf_{y \in \mathbb{R}^{\Lambda(2d)}} \left\{ \langle f, y \rangle;\ y_0 = 1,\ M_{d-v_i}(g_i \cdot y) \succeq 0,\ i = 0, \ldots, m \right\}, \tag{6}$$

relaxed from (5).

For a given $d \geq d_0$, the optimization problem (6) is a semidefinite program (and can then be numerically solved using SDP solvers). Indeed, for all $y \in \mathbb{R}^{\Lambda(2d)}$ such that $y_0 = 1$ and all $i \in \{0, \ldots, m\}$, we can write

$$M_{d-v_i}(g_i \cdot y) = A_{0\,i} + \sum_{\alpha \in \Lambda(2d)\setminus\{0\}} y_\alpha A_{\alpha\,i}$$

where, for all $\alpha \in \Lambda(2d)$, $A_{\alpha\,i}$ is a symmetric square matrix of size $\Lambda(d - v_i)$ (see also [66, section 5]).

The following theorem of Lasserre ([42, Theorem 6.2], see also [66, Theorem 1.5]) asserts that the sequence of optima $(\rho_d)_{d \geq d_0}$ converges to f^*:

Theorem 3.4 (Lasserre)**.** *The sequence $(\rho_d)_{d \geq d_0}$ is a nondecreasing sequence that converges to f^*.*

Proof. Let d be an integer such that $d \geq d_0$ and denote by F_d the set of vectors $y \in \mathbb{R}^{\Lambda(2d)}$ such that $y_0 = 1$ and $M_{d-v_i}(g_i \cdot y) \succeq 0$ for all $i \in \{0, \ldots, m\}$. The set $\{\langle f, y\rangle;\ y \in F_{d+1}\}$ is included in the set $\{\langle f, y\rangle;\ y \in F_d\}$. Indeed, if $y \in F_{d+1}$ and if we denote by $\overline{y}$ the truncation $(y_\alpha)_{\alpha \in \Lambda(2d)}$ of y, we have $\overline{y}_0 = y_0 = 1$ and, for $i \in \{0, \ldots, m\}$, $M_{d-v_i}(g_i \cdot \overline{y}) \succeq 0$ (because $M_{d-v_i}(g_i \cdot \overline{y})$ is a principal submatrix of the positive semidefinite matrix $M_{d+1-v_i}(g_i \cdot y)$), as well as $\langle f, \overline{y}\rangle = \langle f, y\rangle$ since $\deg f \leq 2d$. As a consequence, $\rho_d \leq \rho_{d+1}$.

We then show that the nondecreasing sequence $(\rho_d)_{d \geq d_0}$ is bounded by f^*. Consider the formulation (5) of our optimization problem and denote by F the set of sequences $y \in \mathbb{R}^{\mathbb{N}^n}$ such that $y_0 = 1$ and $M(g_i \cdot y) \succeq 0$ for all $i \in \{0, \ldots, m\}$. Let y be in F and let $\overline{y} := (y_\alpha)_{\alpha \in \Lambda(2d)}$ be the truncation of y. Again, we have $\overline{y}_0 = 1$, $M_{d-v_i}(g_i \cdot \overline{y}) \succeq 0$, $i \in \{0, \ldots, m\}$, and $\langle f, \overline{y}\rangle = \langle f, y\rangle$, so that $\rho_d \leq f^*$. Therefore, the sequence $(\rho_d)_{d \geq d_0}$ converges.

The last step is to show that f^* is actually the limit of $(\rho_d)_{d \geq d_0}$. If ϵ is a positive real number, one can show that there exists $d \geq d_0$ such that $f^* - \epsilon \leq \rho_d \leq f^*$: the interested reader is invited to refer to [42, Theorem 6.2] or [66, Theorem 1.5]. The proof involves the dual SDP associated to (6), together with Putinar's Positivstellensatz 3.3. □

4. Lasserre's algorithm – GloptiPoly

The principle of Lasserre's algorithm to solve problem (2) is to numerically compute the sequence of optima $(\rho_d)_{d \geq d_0}$ (which by theorem 3.4 converges to f^*) using SDP solvers at each step. In order to complete this approach, one has to define a stopping criterion for the algorithm. In [42, section 6.1], Lasserre chooses a sufficient condition in terms of ranks of moment matrices, a condition which is motivated by the theorem below. The result we show is actually a slight generalization of [42, Theorem 6.6], that we decided to state in order to take into account the fact that a SDP solver, when applied to the SDP (6), only provides, at best, a numerical approximation of the optimum ρ_d. Let ϵ be a nonnegative real number, d be an integer such that $d \geq d_0$ and denote $v := \max(v_1, \ldots, v_m)$.

Theorem 4.1. *Let $y \in F_d$ (we defined F_d in the proof of theorem 3.4) such that $\rho_d \leq \langle f, y\rangle \leq \rho_d + \epsilon$. If $\operatorname{rank} M_{d-v}(y) = \operatorname{rank} M_d(y)$ then*

$$f^* \leq \langle f, y\rangle \leq \rho_d + \epsilon \leq f^* + \epsilon.$$

Moreover, if we denote $s := \operatorname{rank} M_d(y)$, there exist at least s points $\boldsymbol{x}$ of K such that $f^* \leq f(\boldsymbol{x}) \leq f^* + \epsilon$.

In other words, if an optimal solution y, up to a fixed precision ϵ, of the SDP (6) satisfies the above rank condition on its moment matrix, then $\langle f, y\rangle$ is an approximation of f^* up to precision ϵ. Furthermore, there exist at least $\operatorname{rank} M_d(y)$ points of K which are global minimizers of f up to precision ϵ.

Remark 4.2. (1) For $\epsilon = 0$, we recover Theorem 6.6 in [42].

(2) The SDP solver used in the algorithm of Lasserre implemented in the freeware *GloptiPoly 3* computes an element y of F_d which is an approximation of an optimal solution of (6) and such that the rank r of $M_d(y)$ is maximal among the ranks of moment matrices of elements of F_d. GloptiPoly then checks if the *numerical rank* of the principal submatrix $M_{d-v}(y)$ of $M_d(y)$ is equal to r. The *numerical rank* of a matrix M is, roughly speaking, the number of singular values of M which are greater than a fixed precision, and the numerical rank of M is not greater than its rank. As a consequence, if the numerical rank of $M_{d-v}(y)$ is (at least) r, we have the inequalities $r \leq \operatorname{rank} M_{d-v}(y) \leq \operatorname{rank} M_d(y) = r$ so that $\operatorname{rank} M_{d-v}(y) = \operatorname{rank} M_d(y)$ and the stopping criterion of theorem 4.1 applies. More details about these questions can be found in [34, sections 4.4.1 and 4.4.2].

(3) In [42, section 6.1.2] is described the algorithm, implemented in GloptiPoly, which extract (approximated) global minimizers of f when the rank condition is satisfied.

Theorem 4.1 is a consequence of the following one whose sketch of proof is postponed below. For any $r \in \mathbb{N}\setminus\{0\}$, a Borel measure μ on $\mathbb{R}^n$ is said to be *r-atomic* if there exist $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_r \in \mathbb{R}^n$ and positive real numbers $\lambda_1, \ldots, \lambda_r$ such that $\mu = \sum_{i=1}^r \lambda_i \delta_{\boldsymbol{x}_i}$.

Theorem 4.3 (Curto–Fialkow [16], Laurent [43])**.** *Let $y \in F_d$. If $\operatorname{rank} M_{d-v}(y) = \operatorname{rank} M_d(y)$, then y can be represented by a s-atomic measure, where $s := \operatorname{rank} M_d(y)$, whose support is included in K.*

Proof of theorem 4.1. We adapt the proof of [42, theorem 6.6]. Suppose that rank $M_{d-v}(y) =$ rank $M_d(y)$. Then, by theorem 4.3, y has a s-atomic representing measure μ with support included in K : there exist $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_s \in K$ and $\lambda_1, \ldots, \lambda_s \in]0; +\infty[$ such that $\mu = \sum_{i=1}^s \lambda_i \delta_{\boldsymbol{x}_i}$. In particular, since $y_0 = 1$, we have $1 = y_0 = \int_{\mathbb{R}^n} \mu(\boldsymbol{x}) = \sum_{i=1}^s \lambda_i$. Then

$$\langle f, y\rangle = \sum_{\alpha\in\Lambda(2d)} f_\alpha y_\alpha = \int_{\mathbb{R}^n} \sum_{\alpha\in\Lambda(2d)} f_\alpha \boldsymbol{x}^\alpha \mathrm{d}\mu(\boldsymbol{x}) = \sum_{i=1}^s \lambda_i f(\boldsymbol{x}_i) \geq \sum_{i=1}^s \lambda_i f^* = f^*,$$

so that $f^* + \epsilon \geq \rho_d + \epsilon \geq \langle f, y\rangle \geq f^*$.

Finally suppose that there exists $i \in \{1, \ldots, s\}$ such that $f(\boldsymbol{x}_i) > f^* + \epsilon$. This implies that

$$\sum_{j=1}^s \lambda_j f(\boldsymbol{x}_j) > \left(\sum_{j=1}^s \lambda_j f^*\right) + \epsilon = f^* + \epsilon,$$

which is not true according to the above inequalities. As a consequence, for all $i \in \{1, \ldots, s\}$, $f^* \leq f(\boldsymbol{x}_i) \leq f^* + \epsilon$. □

Proof of theorem 4.3. We point out the essential steps of the reasoning, referring to [44] for the detailed proofs. We have

$$\operatorname{rank} M_{d-v}(y) \leq \operatorname{rank} M_{d-v+1}(y) \leq \cdots \leq \operatorname{rank} M_{d-1}(y) \leq \operatorname{rank} M_d(y)$$

and suppose that $\operatorname{rank} M_{d-v}(y) = \operatorname{rank} M_d(y)$: we obtain that $\operatorname{rank} M_{d-1}(y) = \operatorname{rank} M_d(y)$. We can then recursively apply the Flat Extension Theorem 5.14 of [44] (originally due to Curto and Fialkow in [15]) to assert the existence of a sequence $\widetilde{y}$ of $\mathbb{R}^{\mathbb{N}^n}$ such that, for all $\alpha \in \Lambda(2d)$, $\widetilde{y}_\alpha = y_\alpha$ and, for all $k \in \mathbb{N}$ satisfying $k \geq d - v$, $\operatorname{rank} M_k(\widetilde{y}) = \operatorname{rank} M_d(y) = s$.

In particular, for all $k \geq d$, since the principal submatrix $M_d(y) = M_d(\widetilde{y})$ of $M_k(\widetilde{y})$ is positive semidefinite (because y is in F_d) and $\operatorname{rank} M_k(\widetilde{y}) = \operatorname{rank} M_d(\widetilde{y})$, the symmetric matrix $M_k(\widetilde{y})$ is also positive semidefinite (see [44, Definition 1.1]). In other words, the (infinite) moment matrix $M(\widetilde{y})$ is positive semidefinite. Since, furthermore, $\operatorname{rank} M(\widetilde{y}) = s$, by [44, Theorem 5.1 (i)], there is a s-atomic measure μ representing $\widetilde{y}$, and then y, with support the finite real algebraic set

$$V(I) := \{\boldsymbol{x} \in \mathbb{R}^n;\ \text{for all } p \in I, p(\boldsymbol{x}) = 0\}$$

where $I := \{p \in \mathbb{R}[X];\ Mp = 0\}$ (the proof of Theorem 5.1 (i) of [44] involves real algebraic geometry).

The last step is then to prove that this support is included in K. Write $V(I) = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_s\}$ and let $\lambda_1, \ldots, \lambda_s \in]0; +\infty[$ such that $\mu = \sum_{i=1}^s \lambda_i \delta_{\boldsymbol{x}_i}$. By Lemma 5.6 of [44], there exist

$p_1, \ldots, p_s \in \mathbb{R}[X]$ of degree at most $d - v$ such that, for all $i, j \in \{1, \ldots, s\}$, $p_i(\boldsymbol{x}_j) = \delta_{ij}$ (see also [44, Lemma 2.3]). For all $i \in \{1, \ldots, s\}$ and $j \in \{1, \ldots, m\}$, we then have, because $y \in F_d$,

$$0 \leq p_i^T M_{d-v}(g_j \cdot y) p_i = \int_{\mathbb{R}^n} g_j(\boldsymbol{x}) p_i(\boldsymbol{x})^2 \mathrm{d}\mu(\boldsymbol{x}) = \sum_{k=1}^{s} \lambda_k g_j(\boldsymbol{x}_k) p_i(\boldsymbol{x}_k)^2 = \lambda_i g_j(\boldsymbol{x}_i)$$

(see the proof of proposition 3.1 above for the first equality) and, since $\lambda_i > 0$, $g_j(\boldsymbol{x}_i) \geq 0$. As a consequence, for all $i \in \{1, \ldots, s\}$, $\boldsymbol{x}_i \in \{\boldsymbol{x} \in \mathbb{R}^n;\ g_1(\boldsymbol{x}) \geq 0, \ldots, g_m(\boldsymbol{x}) \geq 0\} = K$. □

We finally present the algorithm implemented by Lasserre and Henrion in the Matlab freeware *GloptiPoly 3* to numerically solve polynomial optimization problems. For details on GloptiPoly and its use, see [33] and Appendix B of [42].

In order to solve a SDP relaxation ρ_d, $d \geq d_0$, GloptiPoly 3 uses by default the SDP solver SeDuMi of Sturm [70]. Other SDP solvers can also be used as long as they are interfaced through Yalmip [46] (see section 5.9 of [33]).

The inputs of GloptiPoly are

- the variables $X_1, \ldots, X_n$,
- the polynomial $f \in \mathbb{R}[X_1, \ldots, X_n]$,
- the polynomials $g_j \in \mathbb{R}[X_1, \ldots, X_n]$, $j \in \{1, \ldots, m\}$, satisfying the Archimedean hypothesis,
- a maximal relaxation order $d_{\max} \geq d_0$.

The first output is a *status* number $\xi \in \{-1, 0, 1\}$:

- $\xi = -1$ means that the consider SDP solver could not solve numerically any of the relaxations ρ_d, $d \in \{d_0, \ldots, d_{\max}\}$;
- $\xi = 0$ means that the solver numerically solved (that is up to a prescribed precision ϵ) at least one of the relaxations ρ_d, $d \in \{d_0, \ldots, d_{\max}\}$, but at each such success either no optimal solution was provided by the solver, either the rank stopping criterion of Theorem 4.1 was not satisfied by the (approximated up to precision ϵ) obtained optimal solution y_d. In that case, the algorithm also outputs the last computed (and then greatest) optimal value ρ_d which is (up to precision ϵ) a lower bound for f^*;
- $\xi = 1$ means that the rank stopping criterion of Theorem 4.1 has been satisfied by an optimal solution y_d of a solved relaxation ρ_d, $d \in \{d_0, \ldots, d_{\max}\}$. In that case, the algorithm also outputs ρ_d which is then an approximation of f^* up to the prescribed precision ϵ.

Lasserre's algorithm for polynomial optimization is, in pseudo code, the following (see [44, Algorithm 6.1]):

```
d ← d_0
ρ ← −∞
ξ ← −1
while d ≤ d_max do ask SDP solver to solve ρ_d
    if not possible then
        d ← d + 1
    else
        ξ ← 0
        ρ ← optimal value provided by the solver
        if SDP solver found an optimal solution y and y satisfies rank stopping criterion then
            ξ ← +1
            Return ξ,ρ
            Stop
        else
            d ← d + 1
        end if
    end if
end while
```

Return ξ,ρ

Remark 4.4. (1) When the rank condition is satisfied, we can also ask GloptiPoly to extract minimizers up to precision ϵ (in the sense of Theorem 4.1), which involves the algorithm described in [42, section 6.1.2].
(2) If the output ξ is 0 or -1, one can increase $d_{\max}$ to try to obtain an approximation (or a better lower bound) of f^* at a higher relaxation order.
(3) There is no complexity known for Lasserre's method. Actually, we do not know if there is a maximal relaxation degree $d_{\max}$, dependent on the inputs of the problem, which would ensure the rank stopping criterion to be satisfied at some ordre $d \leq d_{\max}$. However, what makes this method advantageous is that it benefits from the interesting complexity of SDP solvers to solve semidefinite programs (see for instance [42] A.1.2).

We conclude this part by the following remark: the convergence of Lasserre's polynomial optimization method, described in the previous sections, takes place when the constraint set is a semialgebraic compact set satisfying the Archimedean property 3.2. Nevertheless, when the Archimedean condition is not satisfied but the polynomial function f is coercive, Jeyakumar–Lasserre–Li in [37] provide a way to consider the optimization problem (2) as a problem with constraints satisfying the Archimedean condition :

Lemma 4.5 (Jeyakumar–Lasserre–Li)**.** *Suppose that the polynomial function $f : \mathbb{R}^n \to \mathbb{R}$ associated to $f \in \mathbb{R}[X_1, \dots, X_n]$ is coercive, and let $c > 0$ and $\boldsymbol{y} \in K$ such that $c > f(\boldsymbol{y})$. Then the quadratic module $\mathbf{M}(g_1, \dots, g_m, c - f)$ associated to the semialgebraic set*

$$\widetilde{K} = \{\boldsymbol{x} \in \mathbb{R}^n;\ g_1(\boldsymbol{x}) \geq 0, \dots, g_m(\boldsymbol{x}) \geq 0, c - f(\boldsymbol{x}) \geq 0\}$$

is Archimedean (in particular, $\widetilde{K}$ is compact). Furthermore,

$$f^* = \inf_{\boldsymbol{x} \in K} f(\boldsymbol{x}) = \inf_{\boldsymbol{x} \in \widetilde{K}} f(\boldsymbol{x}) = \min_{\boldsymbol{x} \in \widetilde{K}} f(\boldsymbol{x}).$$

Proof. The set $E = \{\boldsymbol{x} \in \mathbb{R}^n;\ c - f(\boldsymbol{x}) \geq 0\}$ is not empty since $\boldsymbol{y} \in E$. Furthermore, the set E is compact. Indeed, if we suppose that E is not bounded, we can find a sequence $(x_n)_{n \in \mathbb{N}}$ of elements of E such that $\|x_n\| \to +\infty$. But then $f(x_n) \to +\infty$ since f is coercive, which is impossible since, by definition of E, for all $n \in \mathbb{N}$, $f(x_n) \leq c$. Since $E = \{\boldsymbol{x} \in \mathbb{R}^n;\ c - f(\boldsymbol{x}) \geq 0\}$ is compact, then the quadratic module $\mathbf{M}(g_1, \dots, g_m, c - f)$ is Archimedean by [66, Theorem 1.1]. Finally, we have $c > f(\boldsymbol{y})$ so $c > f^*$ and

$$f^* = \inf\{f(\boldsymbol{x});\ \boldsymbol{x} \in K\} = \inf\{f(\boldsymbol{x});\ \boldsymbol{x} \in K \cap \{c - f \geq 0\}\ \} = \inf\left\{f(\boldsymbol{x});\ \boldsymbol{x} \in \widetilde{K}\right\}.$$

□

In other words, even if the polynomials $g_1, \dots, g_m$ do not satisfy themselves the Archimedean hypothesis, provided that f is coercive, we can place ourselves in the range of application of Lasserre's method by adding the inequality $c - f \geq 0$ to the constraints $g_1 \geq 0, \dots, g_m \geq 0$.

Remark 4.6. In [42, theorem 6.5], Lasserre states some classical conditions (known as the Karush–Kuhn–Tucker (KKT) conditions [42, section 7.1]), already encountered in nonlinear programming, to ensure the finite convergence of the hierarchy of the semidefinite relaxations (6). These conditions are initially a certificate for global optimality [42, theorem 7.4 and 7.5] and hold generically for a polynomial optimization problem [42, theorem 7.6].

5. Distance to the transversely isotropic stratum of the symmetric second-order tensor

Let $\mathbb{V} = \mathbb{S}^2(\mathbb{R}^3)$ be the vector space of symmetric second-order tensors, endowed with the natural action $\rho_2(g)\mathbf{a} = g\,\mathbf{a}\,g^T$, for $\mathbf{a} \in \mathbb{S}^2(\mathbb{R}^3)$, $g \in G = \mathrm{SO}(3)$. Let $\mathbf{q} = (\delta_{ij})$ be the *Euclidean metric*,

$$\mathbf{a}' = \mathbf{a} - \frac{1}{3}\,\mathrm{tr}(\mathbf{a})\,\mathbf{q},$$

be the *traceless part* of $\mathbf{a}$, $\boldsymbol{\varepsilon}$ be the *Levi-Civita* tensor. We denote by $(\,)^s$ the *total symmetrization* of a tensor. The generalized cross-product of symmetric tensors is defined as [61]

$$\mathbf{a} \times \mathbf{b} := -(\mathbf{a} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{b})^s, \qquad (i.e.,\ (\mathbf{a} \times \mathbf{b})_{ijk} := -(a_{il}\varepsilon_{ljs}b_{sk})^s)\,. \tag{7}$$

For $\mathbf{a}, \mathbf{b} \in \mathbb{S}^2(\mathbb{R}^3)$, it is a totally symmetric third-order tensor with 10 independent components.

There are three isotropy classes for the symmetric second-order tensors $(\mathbb{S}^2(\mathbb{R}^3), \mathrm{SO}(3))$:

- $[\mathbb{D}_2]$ (orthotropy), if $\mathbf{a}$ has three distinct eigenvalues,
- $[\mathrm{O}(2)]$ (transverse isotropy, characterized by the polynomial equation $\mathbf{a}^2 \times \mathbf{a} = 0$ [61, Lemma 8.1]), if $\mathbf{a}$ has two distinct eigenvalues.
- $[\mathrm{SO}(3)]$ (isotropy, characterized by the linear equation $\mathbf{a}' = 0$), if $\mathbf{a}$ has three equal eigenvalues.

We illustrate through this first example the accuracy of Lasserre's polynomial optimization method to compute the *distance to an isotropy stratum*. We shall obtain by this way the distance $\Delta(\mathbf{a}_0, \overline{\Sigma}_{[\mathrm{O}(2)]})$ of the orthotropic second-order tensor

$$\mathbf{a}_0 = \begin{pmatrix} -7 & 4 & -4 \\ 4 & 5 & -2 \\ -4 & -2 & 5 \end{pmatrix}$$

and compare the numerical results obtained with the algebraic solution derived in [4]:

$$\Delta(\mathbf{a}_0, \overline{\Sigma}_{[\mathrm{O}(2)]})^2 = \|\mathbf{a}_0 - \mathbf{a}^{**}\|^2 = 18, \tag{8}$$

where

$$\mathbf{a}^{**} = \frac{1}{6}\begin{pmatrix} -44 & 20 & -20 \\ 20 & 31 & 5 \\ -20 & 5 & 31 \end{pmatrix} \approx \begin{pmatrix} -7.333333 & 3.333333 & -3.333333 \\ 3.333333 & 5.166667 & 0.8333333 \\ -3.333333 & 0.8333333 & 5.166667 \end{pmatrix}. \tag{9}$$

The numerical problem is first reduced to the following polynomial optimization problem

$$\min_{\mathbf{a} \in K} \|\mathbf{a}_0 - \mathbf{a}\|^2,$$

where

$$K = \left\{\mathbf{a};\ \mathbf{a}^2 \times \mathbf{a} = 0\right\}.$$

Then, in order to properly apply the algorithm described in section 4, we need to ensure the Archimedean property (definition 3.2), and for that we use lemma 4.5. Therefore, to the 10 equations $\mathbf{a}^2 \times \mathbf{a} = 0$, we add the inequality $c - \|\mathbf{a}_0 - \mathbf{b}\|^2 \geq 0$ where we take

$$\mathbf{b} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \in K,$$

and choose accordingly $c = 300$. GloptiPoly then computes the approximation

$$\|\mathbf{a}_0 - \mathbf{a}^*\|^2 \tag{10}$$

of the minimum $\Delta(\mathbf{a}_0, \overline{\Sigma}_{[\mathrm{O}(2)]})^2 = \min_{\mathbf{a} \in \widetilde{K}} \|\mathbf{a}_0 - \mathbf{a}\|^2$, where

$$\widetilde{K} = \left\{\mathbf{a};\ \mathbf{a}^2 \times \mathbf{a} = 0, c - \|\mathbf{a}_0 - \mathbf{a}\|^2 \geq 0\right\}. \tag{11}$$

The optimal result computed in 1.2 seconds on a standard PC,

$$\Delta(\mathbf{a}_0, \overline{\Sigma}_{[\mathrm{O}(2)]})^2 \approx 18.000007, \qquad \mathbf{a}^{**} \approx \mathbf{a}^* = \begin{pmatrix} -7.33299 & 3.33348 & -3.33348 \\ 3.33348 & 5.16651 & 0.83343 \\ -3.33348 & 0.83343 & 5.16651 \end{pmatrix},$$

is close to the exact solution (8)–(9), with the constraints accurately satisfied:

$$\frac{\max_i |g_i(\mathbf{a}^*)|}{\|\mathbf{a}_0\|^3} = \frac{\max_{p,q,r} |(\mathbf{a}^{*\,2} \times \mathbf{a}^*)_{pqr}|}{\|\mathbf{a}_0\|^3} = 5.696\,10^{-9}.$$

For different values $c \in [202, 450]$, one gets

$$18.000007 \leq \Delta(\mathbf{a}_0, \Sigma_{[\mathrm{O}(2)]})^2 \leq 18.00006,$$

with the GloptiPoly convergence obtained for the first degree of relaxation $d = d_0 = 2$. The value chosen for c affects the numerical solution. In fact, by increasing c we get closer to the true minimum (=18), but the convergence is lost for $c \geq 500$ (with a GloptiPoly status $\xi = 0$ at the first relaxation).

Remark 5.1. The transversely isotropic closed stratum $\overline{\Sigma}_{[\mathrm{O}(2)]}$ can also be characterized by a single scalar equation of degree 6,

$$g(\mathbf{a}) = 12\|\mathbf{a}^2 \times \mathbf{a}\|^2 = \left(\mathrm{tr}(\mathbf{a}'^2)\right)^3 - 6\left(\mathrm{tr}(\mathbf{a}'^3)\right)^2 = 0, \tag{12}$$

with $\mathbf{a}'$, the traceless part of $\mathbf{a}$. However, there is no finite convergence of the associated relaxation problem, since $\mathrm{grad}_{\mathbf{a}}\, g(\mathbf{a}) = \frac{6g(\mathbf{a})}{\mathrm{tr}(\mathbf{a}'^2)}\mathbf{a}' = 0$ when $g(\mathbf{a}) = 0$. In particular, the independence of the gradients of the constraint functions at the minimum (first order KKT sufficient condition mentioned in [42, theorem 6.5, theorem 7.2], see remark 4.6) is not satisfied.

The present example illustrates the strong dependence of the GloptiPoly convergence issue on the characterization of the isotropy classes. Indeed, convergence is obtained for the covariant characterization $\mathbf{a}^2 \times \mathbf{a} = 0$, but not for the invariant characterization (12).

6. Distance to cubic elasticity isotropy stratum

In this section, we compute the distance of an experimental elasticity tensor $\mathbf{E}_0$ to the cubic isotropy stratum $\overline{\Sigma}_{[\mathbb{O}]}$, and determine the associated minimizer $\mathbf{E}^*$. The distance to an isotropy stratum problem has been widely addressed in the Continuum Mechanics literature, by solving it in terms of an unknown rotation (either parameterized by Euler angles [24, 25], or by a unit quaternion [18, 38, 39]). Here, we use the characterization of the (cubic) isotropy stratum by means of at most quadratic covariants in order to formulate such a distance problem as a quadratic polynomial optimization problem. This makes us able to apply Lasserre's method, and to show that using GloptiPoly allows to compute an accurate solution of this non trivial example.

6.1. Formulation of the distance problem as a polynomial optimization problem.

Let

$$\mathbb{V} = \mathbb{E}\mathrm{la} = \left\{\mathbf{E} \in \otimes^4\mathbb{R}^3,\ E_{ijkl} = E_{jikl} = E_{klij}\right\} \qquad (\dim \mathbb{E}\mathrm{la} = 21)$$

be the set of elasticity tensors $\mathbf{E} : \mathbb{S}^2(\mathbb{R}^3) \to \mathbb{S}^2(\mathbb{R}^3)$, introduced in example 2.1, and $G = \mathrm{SO}(3)$. An *elasticity tensor* $\mathbf{E} \in \mathbb{E}\mathrm{la}$ can be represented by a 6×6 symmetric matrix, in Voigt notation,

$$[\mathbf{E}] = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & E_{1123} & E_{1113} & E_{1112} \\ E_{1122} & E_{2222} & E_{2233} & E_{2223} & E_{1223} & E_{1222} \\ E_{1133} & E_{2233} & E_{3333} & E_{2333} & E_{1333} & E_{1233} \\ E_{1123} & E_{2223} & E_{2333} & E_{2323} & E_{2331} & E_{2312} \\ E_{1113} & E_{1223} & E_{1333} & E_{2331} & E_{1313} & E_{3112} \\ E_{1112} & E_{1222} & E_{1233} & E_{2312} & E_{3112} & E_{1212} \end{pmatrix}. \tag{13}$$

The vector space $\mathbb{E}\mathrm{la}$ decomposes into a direct sum of SO(3)-irreducible subspaces (so-called harmonic decomposition [7, 68])

$$\mathbb{E}\mathrm{la} = \mathbb{H}^0(\mathbb{R}^3) \oplus \mathbb{H}^0(\mathbb{R}^3) \oplus \mathbb{H}^2(\mathbb{R}^3) \oplus \mathbb{H}^2(\mathbb{R}^3) \oplus \mathbb{H}^4(\mathbb{R}^3),$$

where $\mathbb{H}^n(\mathbb{R}^3)$ denotes the space of harmonic tensors of order n ($\dim \mathbb{H}^n(\mathbb{R}^3) = 2n+1$). Letting

$$\mathbf{d} = \mathrm{tr}_{12}\,\mathbf{E}, \qquad \mathbf{v} = \mathrm{tr}_{13}\,\mathbf{E},$$

the harmonic decomposition of $\mathbf{E} \in \mathbb{E}\mathrm{la}$ can be expressed as (see Appendix A for explicit formulas)

$$\mathbf{E} = (\alpha, \beta, \mathbf{d}', \mathbf{v}', \mathbf{H}),$$

with $\alpha = \mathrm{tr}\,\mathbf{d}, \beta = \mathrm{tr}\,\mathbf{v} \in \mathbb{H}^0(\mathbb{R}^3)$ the scalar (isotropic) components of $\mathbf{E}$, with $\mathbf{d}', \mathbf{v}' \in \mathbb{H}^2(\mathbb{R}^3)$ its second-order harmonic components (the traceless parts of $\mathbf{d}$ and $\mathbf{v}$), and $\mathbf{H} \in \mathbb{H}^4(\mathbb{R}^3)$ its fourth-order harmonic component. The squared Euclidean norm of $\mathbf{E}$ is then

$$\|\mathbf{E}\|^2 = 5\alpha^2 + 4\beta^2 + \frac{2}{21}\|\mathbf{d}' + 2\mathbf{v}'\|^2 + \frac{4}{3}\|\mathbf{d}' - \mathbf{v}'\|^2 + \|\mathbf{H}\|^2. \tag{14}$$

We consider the triclinic experimental elasticity tensor $\mathbf{E}_0$ representing the Nickel-based aeronautics single crystal superalloy (of CMSX-4 type), measured in [25]. In Voigt notation:

$$[\mathbf{E}_0] = \begin{pmatrix} 243 & 136 & 135 & 22 & 52 & -17 \\ 136 & 239 & 137 & -28 & 11 & 16 \\ 135 & 137 & 233 & 29 & -49 & 3 \\ 22 & -28 & 29 & 133 & -10 & -4 \\ 52 & 11 & -49 & -10 & 119 & -2 \\ -17 & 16 & 3 & -4 & -2 & 130 \end{pmatrix} \text{ GPa.} \tag{15}$$

This material has an expected symmetry, namely the cubic symmetry $[\mathbb{O}]$, deduced from its cubic microstructure (see figure 1).

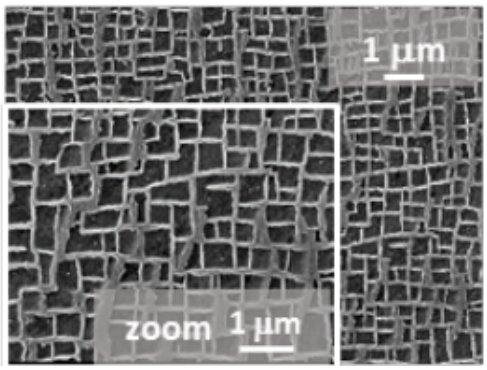

FIGURE 1. Cubic microstructure of CMSX-4 Ni-based single crystal superalloy [51].

We then aim a computing of

$$\Delta(\mathbf{E}_0, \overline{\Sigma}_{[\mathbb{O}]})^2 = \min_{\mathbf{E}\in\overline{\Sigma}_{\mathbb{O}}} \|\mathbf{E}_0 - \mathbf{E}\|^2. \tag{16}$$

This optimization problem has 21 variables E_{ijkl}. To set it as a polynomial optimization problem, we take advantage of the fact that the cubic elasticity stratum is an algebraic set, characterized by explicit polynomial equations.

Theorem 6.1 (Olive et al [61])**.** *Let* $\mathbf{E} = (\alpha, \beta, \mathbf{d}', \mathbf{v}', \mathbf{H}) \in \mathbb{E}\mathrm{la}$ *be an elasticity tensor,*

$$\mathbf{d}_2 = \mathbf{H} \,\vdots\, \mathbf{H} \qquad (i.e.,\ (\mathbf{d}_2)_{ij} = H_{ipqr}H_{pqrj})$$

and $\mathbf{d}_2' = \mathbf{d}_2 - \frac{1}{3}\operatorname{tr}(\mathbf{d}_2)\,\mathbf{q}$ *be second-order covariants of* $\mathbf{E}$*. Then* $\mathbf{E} \in \overline{\Sigma}_{[\mathbb{O}]}$ *(is at least cubic) if and only if*

$$\mathbf{v}' = \mathbf{d}' = 0 \quad \textit{and} \quad \mathbf{d}_2' = 0,$$

and $\mathbf{E} \in \Sigma_{[\mathbb{O}]}$ *(is cubic) if and only if furthermore* $\mathbf{H} \neq 0$*.*

We have then the following result.

Theorem 6.2. *Let* $\mathbf{E} = (\alpha, \beta, \mathbf{d}', \mathbf{v}', \mathbf{H})$ *and* $\mathbf{E}_0 = (\alpha_0, \beta_0, \mathbf{d}_0', \mathbf{v}_0', \mathbf{H}_0)$ *be two elasticity tensors. The 21-dimensional minimization problem* (16) *is equivalent to the 9-dimensional polynomial optimization problem*

$$\min_{\mathbf{d}_2'=0} \|\mathbf{H}_0 - \mathbf{H}\|^2,$$

with $\mathbf{E} = (\alpha_0, \beta_0, 0, 0, \mathbf{H})$*, and*

$$\min_{\mathbf{E}\in\overline{\Sigma}_{\mathbb{O}}} \|\mathbf{E}_0 - \mathbf{E}\|^2 = \frac{2}{21}\|\mathbf{d}_0' + 2\mathbf{v}_0'\|^2 + \frac{4}{3}\|\mathbf{d}_0' - \mathbf{v}_0'\|^2 + \min_{\mathbf{d}_2'=0}\|\mathbf{H}_0 - \mathbf{H}\|^2. \tag{17}$$

Proof. The squared distance function in (16) is

$$\|\mathbf{E}_0 - \mathbf{E}\|^2 = \|(\alpha_0 - \alpha, \beta_0 - \beta, \mathbf{d}_0' - \mathbf{d}', \mathbf{v}_0' - \mathbf{v}', \mathbf{H}_0 - \mathbf{H})\|^2.$$

It can be expressed as

$$\|\mathbf{E}_0-\mathbf{E}\|^2 = 5(\alpha_0-\alpha)^2+4(\beta_0-\beta)^2+\frac{2}{21}\|\mathbf{d}_0'+2\mathbf{v}_0'-(\mathbf{d}'+2\mathbf{v}')\|^2+\frac{4}{3}\|\mathbf{d}_0'-\mathbf{v}_0'-(\mathbf{d}'-\mathbf{v}')\|^2+\|\mathbf{H}_0-\mathbf{H}\|^2,$$

by using (14). By theorem 6.1, taking $\alpha = \alpha_0$, $\beta = \beta_0$, $\mathbf{d}' = 0$ and $\mathbf{v}' = 0$, we get (17), and the polynomial optimization problem (16) is reduced to the following problem in only 9 variables (the components of $\mathbf{H} \in \mathbb{H}^4(\mathbb{R}^3)$, $\dim \mathbb{H}^4(\mathbb{R}^3) = 9$) instead of 21,

$$\min_{\mathbf{d}_2'=0} \|\mathbf{H}_0 - \mathbf{H}\|^2.$$

□

Remark 6.3. An elasticity tensor $\mathbf{E} \in \mathbb{E}\mathrm{la}$ corresponds to a quadratic elastic energy density, which must be positive semidefinite. This condition can be characterized using SO(3)-invariant polynomial inequalities on $\mathbf{E}$, and thus added to the set of polynomial constraints, if necessary, using the following fact. Given a symmetric real $n \times n$ matrix A, we get

$$A \text{ is positive semidefinite} \iff \forall i \in \{1, \dots, n\}\,,\ \sigma_i \geq 0,$$

where $\sigma_1, \dots, \sigma_n$ denote the elementary symmetric polynomials in the eigenvalues λ_i of A. Indeed, if $\lambda_i \geq 0$ for all $i \in \{1, \dots, n\}$, then $\sigma_i \geq 0$ for all $i \in \{1, \dots, n\}$. Conversely, assume that $\sigma_i \geq 0$ for all $i \in \{1, \dots, n\}$. Then, the polynomial

$$p := (X + \lambda_1)(X + \lambda_2) \dots (X + \lambda_n) = X^n + \sigma_1 X^{n-1} + \dots + \sigma_{n-1} X + \sigma_n,$$

satisfies

$$p(x) \geq x^n > 0, \qquad \forall x > 0.$$

Hence, the (real) roots of p, namely $-\lambda_1, \dots, -\lambda_n$, belong to $]-\infty, 0]$, and thus $\lambda_i \geq 0$ for all $i \in \{1, \dots, n\}$.

In practice, an experimental tensor $\mathbf{E}_0$ is most often measured as semidefinite and the tensor the closest to $\mathbf{E}_0$ computed as semidefinite, so, here we do not add the semidefiniteness constraint $\mathbf{E} \geq 0$ to our optimization problem.

6.2. **Resolution by Lasserre's method.** A fourth order harmonic tensor $\mathbf{H} \in \mathbb{H}^4(\mathbb{R}^3)$ is represented by the following real matrix (in Voigt notation)

$$[\mathbf{H}] = \begin{pmatrix} \Lambda_2+\Lambda_3 & -\Lambda_3 & -\Lambda_2 & -X_1 & Y_1+Y_2 & -Z_2 \\ -\Lambda_3 & \Lambda_3+\Lambda_1 & -\Lambda_1 & -X_2 & -Y_1 & Z_1+Z_2 \\ -\Lambda_2 & -\Lambda_1 & \Lambda_1+\Lambda_2 & X_1+X_2 & -Y_2 & -Z_1 \\ -X_1 & -X_2 & X_1+X_2 & -\Lambda_1 & -Z_1 & -Y_1 \\ Y_1+Y_2 & -Y_1 & -Y_2 & -Z_1 & -\Lambda_2 & -X_1 \\ -Z_2 & Z_1+Z_2 & -Z_1 & -Y_1 & -X_1 & -\Lambda_3 \end{pmatrix}. \tag{18}$$

In practice we set

$$\boldsymbol{x} = (\Lambda_1, \Lambda_2, \Lambda_3, X_1, X_2, Y_1, Y_2, Z_1, Z_2),$$

and GloptiPoly computes the approximation

$$\|\mathbf{H}_0 - \mathbf{H}^*\|^2 \tag{19}$$

of the minimum $\Delta(\mathbf{H}_0, \overline{\Sigma}_{[\mathbb{O}]})^2 = \min_{\boldsymbol{x} \in \widetilde{K}} f(\boldsymbol{x})$, where $f(\boldsymbol{x}) = \|\mathbf{H}_0 - \mathbf{H}\|^2$ and

$$\widetilde{K} = \left\{\boldsymbol{x};\ \mathbf{d}_2' = 0,\ c - f(\boldsymbol{x}) \geq 0\right\},$$

with $c = 58000 > f(0)$ to ensure the Archimedean property on the set of constraints. The five quadratic scalar equations $(\mathbf{d}_2')_{ij} = 0$ are detailed in Appendix B. For $\mathbf{E}_0$ given by (15), we have

$$\begin{aligned} f(\boldsymbol{x}) = {} & 540\Lambda_2 + 620\Lambda_3 - 88X_1 + 668\Lambda_1 - 264Z_1 - 264Z_2 - 456X_2 + 8Z_2^2 + 8\Lambda_1^2 \\ & + 8\Lambda_2^2 + 8\Lambda_3^2 + 8Y_2^2 + 16X_1^2 + 8X_2^2 + 16Y_1^2 + 16Z_1^2 - 392Y_1 - 808Y_2 \\ & + 8Z_1Z_2 + 2\Lambda_1\Lambda_2 + 2\Lambda_2\Lambda_3 + 8X_1X_2 + 8Y_1Y_2 + 2\Lambda_3\Lambda_1 + \frac{2026042}{35}. \end{aligned}$$

We obtain the result at the first relaxation order $d = d_0 = 1$ with GloptiPoly status $\xi = +1$ and value

$$\min_{\boldsymbol{x} \in \widetilde{K}} f(\boldsymbol{x}) \approx \; f(\boldsymbol{x}^*) = 2530.474727 \text{ GPa}^2,$$

The computation time is of 0.9 seconds. The computed minimizer is

$$\boldsymbol{x}^* = (-36.401489, -20.227012, -38.908985, -6.396664, 27.780748, \\ -2.277546, 44.251364, -4.557344, 21.161507).$$

By (18), it corresponds to the fourth-order harmonic tensor $\mathbf{H}^*$ solution of (19).

We get, by theorem 6.2, $\mathbf{E}^* = (\alpha_0, \beta_0, 0, 0, \mathbf{H}^*)$, *i.e.*,

$$\mathbf{E}^* = \frac{1}{15}(\alpha_0 + 2\beta_0)\,\mathbf{q} \odot \mathbf{q} + \frac{1}{6}(\alpha_0 - \beta_0)\,\mathbf{q} \underset{(2,2)}{\otimes} \mathbf{q} + \mathbf{H}^*,$$

with $\odot$ the symmetric tensor product (see Appendix A). The elasticity tensor $\mathbf{E}^*$ is cubic (and not isotropic) since $\mathbf{H}^* \neq 0$.

Finally, the computed cubic tensor $\mathbf{E}^* \in \Sigma_{[\mathbb{O}]}$ the closest to $\mathbf{E}_0$ is, in Voigt notation,

$$[\mathbf{E}^*] = \begin{pmatrix} 240.130669 & 144.442318 & 125.760345 & 6.39666 & 41.97381 & -21.161507 \\ 144.442318 & 223.956191 & 141.934823 & -27.780748 & 2.277546 & 16.604162 \\ 125.760345 & 141.934823 & 242.638164 & 21.384084 & -44.251364 & 4.557344 \\ 6.39666 & -27.780748 & 21.384084 & 133.268156 & 4.557344 & 2.277546 \\ 41.973817 & 2.277546 & -44.251364 & 4.557344 & 117.093678 & 6.39666 \\ -21.161507 & 16.604162 & 4.557344 & 2.277546 & 6.39666 & 135.775651 \end{pmatrix} \text{ GPa}.$$

It corresponds to $\Delta(\mathbf{E}_0, \overline{\Sigma}_{[\mathbb{O}]}) \approx \|\mathbf{E}_0 - \mathbf{E}^*\| = 74.131148$ GPa and to the relative distance to cubic symmetry

$$\frac{\|\mathbf{E}_0 - \mathbf{E}^*\|}{\|\mathbf{E}_0\|} = 0.103910,$$

slightly better than the solution computed in [25] using a parameterization by Euler angles together with a simplex minimization method. Note that the constraint $\mathbf{d}_2' = 0$ is satisfied accurately, since

$$\frac{\mathbf{d}_2'}{\|\mathbf{H}_0\|^2} = 10^{-6} \begin{pmatrix} -4.097 & -2.8\ 10^{-6} & -4.9\ 10^{-6} \\ -2.8\ 10^{-6} & -4.455 & 4.2\ 10^{-6} \\ -4.9\ 10^{-6} & 4.2\ 10^{-6} & -8.552 \end{pmatrix} \approx \mathbf{0}.$$

One can choose other values for c satisfying $c > f(\boldsymbol{y})$ for some $\boldsymbol{y} \in K$. The GloptiPoly solution varies slightly as c runs the interval $[58000, 61000]$, with a computation time of 0.9 seconds for $c = 58000$, of 0.8 seconds for $c = 60000$, and of 0.1 seconds for $c = 61000$. Outside from this narrow interval, the GloptiPoly convergence is lost (Gloptipoly status $\xi = 0$).

Remark 6.4. The computation time is lower for this quadratic optimization problem (with 9 variables) than for the degree 3 polynomial optimization problem of section 5 (with 6 variables).

7. Distance to cubic piezoelectricity isotropy stratum

In this final section, we apply Lasserre's polynomial optimization method to compute the distance $\Delta(\mathbf{e}_0, \overline{\Sigma}_{[\mathbb{O}^-]})$ of a raw piezoelectricity third-order tensor[1] $\mathbf{e}_0$ to the cubic piezoelectricity stratum $\overline{\Sigma}_{[\mathbb{O}^-]}$. This problem seems to have never been addressed before. It is important for the design of dielectric materials, since for instance the piezolectricity behavior strongly depends on the crystal primitive cell symmetry.

[1]relating induced polarization in a dielectric material to the strain tensor.

7.1. **Formulation of the distance problem as a polynomial optimization problem.** According to the three-dimensional piezoelectricity framework [21, 28], we denote by

$$\mathbb{V} = \mathbb{P}\mathrm{iez} = \left\{\mathbf{e} \in \otimes^3\mathbb{R}^3,\ \mathrm{e}_{ijk} = \mathrm{e}_{ikj}\right\} \qquad (\dim \mathbb{P}\mathrm{iez} = 18),$$

the vector space of piezoelectricity tensors $\mathbf{e} : \mathbb{S}^2(\mathbb{R}^3) \to \mathbb{R}^3$ (see example 2.2), and set $G = \mathrm{O}(3)$. A *piezoelectricity tensor* $\mathbf{e} \in \mathbb{P}\mathrm{iez}$ can be represented by a 3×6 matrix, in so-called Voigt representation,

$$[\mathbf{e}] = \begin{pmatrix} \mathrm{e}_{111} & \mathrm{e}_{122} & \mathrm{e}_{133} & \mathrm{e}_{123} & \mathrm{e}_{113} & \mathrm{e}_{112} \\ \mathrm{e}_{211} & \mathrm{e}_{222} & \mathrm{e}_{233} & \mathrm{e}_{223} & \mathrm{e}_{213} & \mathrm{e}_{212} \\ \mathrm{e}_{311} & \mathrm{e}_{322} & \mathrm{e}_{333} & \mathrm{e}_{323} & \mathrm{e}_{313} & \mathrm{e}_{312} \end{pmatrix}.$$

The vector space $\mathbb{P}\mathrm{iez}$ decomposes into a direct sum of $\mathrm{O}(3)$-irreducible subspaces (so-called harmonic decomposition [68])

$$\mathbb{P}\mathrm{iez} = \mathbb{H}^1(\mathbb{R}^3) \oplus \mathbb{H}^1(\mathbb{R}^3) \oplus \mathbb{H}^{2\sharp}(\mathbb{R}^3) \oplus \mathbb{H}^3(\mathbb{R}^3).$$

The notation $\mathbb{H}^n(\mathbb{R}^3)$ still refers to the vector space of n-th order harmonic tensors endowed with the standard $\mathrm{O}(3)$-representation ρ_n, while $\mathbb{H}^{n\sharp}(\mathbb{R}^3)$ refers to the same vector space endowed with the *twisted* $\mathrm{O}(3)$-representation $\hat{\rho}_n$, such that $\hat{\rho}_n(g) = (\det g)\, \rho_n(g)$. One has

$$\mathbf{e} = (\boldsymbol{v}, \boldsymbol{w}, \mathbf{a}, \mathbf{h})$$

with $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{H}^1(\mathbb{R}^3)$, $\mathbf{a} \in \mathbb{H}^{2\sharp}(\mathbb{R}^3)$ and $\mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$.

Let $\odot$ be the symmetric tensor product and $\mathbf{e}^s \in \mathbb{S}^3(\mathbb{R}^3)$ denote the totally symmetric part of $\mathbf{e}$ (of components $(\mathbf{e}^s)_{ijk} = \frac{1}{3}(\mathrm{e}_{ijk} + \mathrm{e}_{jik} + \mathrm{e}_{kji})$). Any piezoelectricity tensor $\mathbf{e} \in \mathbb{P}\mathrm{iez}$ can be decomposed as the sum

$$\mathbf{e} = \mathbf{g} + \mathbf{h}$$

where

$$\mathbf{h} := \mathbf{e}^s - \frac{3}{5}\mathbf{q} \odot \mathrm{tr}(\mathbf{e}^s) \in \mathbb{H}^3(\mathbb{R}^3), \tag{20}$$

is the *leading harmonic part* of $\mathbf{e}$, and

$$\mathbf{g} := \mathbf{e} - \mathbf{h} = (\boldsymbol{v}, \boldsymbol{w}, \mathbf{a}),$$

is orthogonal to $\mathbf{h}$ (*i.e.*, $\langle \mathbf{g}, \mathbf{h} \rangle = g_{ijk}h_{ijk} = 0$).

Remark 7.1. The third-order tensors $\mathbf{g} = \mathbf{g}(\mathbf{e})$ and $\mathbf{h} = \mathbf{h}(\mathbf{e})$ are linear covariants of $\mathbf{e}$.

The squared Euclidean norm of $\mathbf{e}$ is then

$$\|\mathbf{e}\|^2 = \mathrm{e}_{ijk}\mathrm{e}_{ijk} = \|\mathbf{g}\|^2 + \|\mathbf{h}\|^2. \tag{21}$$

We will first consider the following raw (triclinic) piezoelectricity tensor $\mathbf{e}_0$ for pure wurtzite AlN (aluminum nitride, $x = 0$), of Voigt representation,

$$[\mathbf{e}_0] = \begin{pmatrix} 0 & 0 & -0.0505 & -0.0394 & -0.2854 & -0.0637 \\ -0.0637 & -0.0042 & 0.0332 & -0.2818 & -0.0058 & 0.0185 \\ -0.5807 & -0.5822 & 1.4607 & 0.0022 & 0.0002 & 0.0043 \end{pmatrix} \mathrm{C/m}^2, \tag{22}$$

in Coulomb per square meter, computed by Density Functional Theory (DFT), using ab-initio simulations, by Manna and coworkers [49, Fig.3]. We will also consider wurtzite alloys $\mathrm{Cr}_x\mathrm{Al}_{1-x}\mathrm{N}$ and the associated raw piezoelectricity tensors $\mathbf{e}_0^x$ (given in the Appendix D for chromium concentrations $0 \leq x \leq 0.25$). Note that pure rocksalt CrN corresponds to a Cr-concentration $x = 1$, and that the value $x = 0.25$ is the so-called wurzite to rocksalt phase transition point [52].

We aim at computing by polynomial optimization

$$\Delta(\mathbf{e}_0, \overline{\Sigma}_{[\mathbb{O}^-]})^2 = \min_{\mathbf{e} \in \overline{\Sigma}_{\mathbb{O}^-}} \|\mathbf{e}_0 - \mathbf{e}\|^2, \tag{23}$$

and $\mathbf{e}^* \in \Sigma_{[\mathbb{O}^-]}$ the closest to $\mathbf{e}_0$. In order to succeed, we first have to characterize the cubic piezoelectricity stratum $\overline{\Sigma}_{[\mathbb{O}^-]}$ by polynomial equations (a proof of the following theorem is provided in Appendix C).

Theorem 7.2. *Let* $\mathbf{e} = \mathbf{g} + \mathbf{h} \in \mathbb{P}\mathrm{iez}$ *be a piezoelectricity tensor, with* $\mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$ *its leading harmonic part, let*

$$\mathbf{d}_2 = \mathbf{h} : \mathbf{h} \qquad (\text{i.e., } (\mathbf{d}_2)_{ij} = h_{ikl}h_{klj}),$$

and $\mathbf{d}_2' = \mathbf{d}_2 - \frac{1}{3}\operatorname{tr}(\mathbf{d}_2)\,\mathbf{q}$ *be second-order covariants of* $\mathbf{e}$. *Then* $\mathbf{e} \in \overline{\Sigma}_{[\mathbb{O}^-]}$ *(is at least cubic) if and only if*

$$\mathbf{g} = 0 \quad \textit{and} \quad \mathbf{d}_2' = 0,$$

and $\mathbf{e} \in \Sigma_{[\mathbb{O}^-]}$ *(is cubic) if and only if furthermore* $\mathbf{h} \neq 0$.

With the same proof as for theorem 6.2, we have the following result.

Theorem 7.3. *Let* $\mathbf{e} = \mathbf{g} + \mathbf{h}$ *and* $\mathbf{e}_0 = \mathbf{g}_0 + \mathbf{h}_0$ *be two piezoelectricity tensors, with* $\mathbf{h}$ *and* $\mathbf{h}_0$ *their leading harmonic parts. The 15-dimensional minimization problem* (23) *is equivalent to the 7-dimensional polynomial optimization problem*

$$\min_{\mathbf{d}_2'=0} \|\mathbf{h}_0 - \mathbf{h}\|^2,$$

with $\mathbf{e} = \mathbf{h}$, *and*

$$\min_{\mathbf{e}\in\overline{\Sigma}_{\mathbb{O}^-}} \|\mathbf{e}_0 - \mathbf{e}\|^2 = \|\mathbf{g}_0\|^2 + \min_{\mathbf{d}_2'=0} \|\mathbf{h}_0 - \mathbf{h}\|^2.$$

7.2. **Resolution by Lasserre's method.** A third order harmonic tensor $\mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$ has seven independent components and is represented by the following real matrix (in Voigt notation)

$$[\mathbf{h}] = \begin{pmatrix} h_{111} & h_{122} & -h_{111} - h_{122} & h_{123} & -h_{223} - h_{333} & h_{112} \\ h_{112} & h_{222} & -h_{112} - h_{222} & h_{223} & h_{123} & h_{122} \\ -h_{223} - h_{333} & h_{223} & h_{333} & -H_{112} - h_{222} & -h_{111} - h_{122} & h_{123} \end{pmatrix} \tag{24}$$

The traceless second order tensor $\mathbf{d}_2'$ has five independent components $(\mathbf{d}_2')_{ij}$ detailed in Appendix B.

We set

$$\boldsymbol{x} = (h_{111},\, h_{112},\, h_{122},\, h_{123},\, h_{222},\, h_{223},\, h_{333}).$$

GloptiPoly computes the approximation

$$\|\mathbf{h}_0 - \mathbf{h}^*\|^2 \tag{25}$$

of the minimum $\Delta(\mathbf{e}_0, \overline{\Sigma}_{[\mathbb{O}^-]})^2 = \min_{\boldsymbol{x}\in\widetilde{K}} f(\boldsymbol{x})$, where $f(\boldsymbol{x}) = \|\mathbf{h}_0 - \mathbf{h}\|^2$ and

$$\widetilde{K} = \left\{\boldsymbol{x};\ \mathbf{d}_2' = 0,\, c - f(\boldsymbol{x}) \geq 0\right\}, \qquad c = 3.$$

For $\mathbf{e}_0$ given by (22), we have (in $\mathrm{C}^2/\mathrm{m}^4$)

$$\begin{aligned} f(\boldsymbol{x}) = {} & 6h_{111}h_{122} + 6h_{223}h_{333} + 6h_{112}h_{222} + 4h_{111}^2 + 6h_{112}^2 + 6h_{122}^2 + 4h_{222}^2 \\ & + 6h_{223}^2 + 4h_{333}^2 + 6h_{123}^2 - 0.1002h_{111} - 0.1742h_{122} + 0.1636h_{123} \\ & - 0.0114h_{223} - 5.2244h_{333} + 0.4574h_{112} + 0.0836h_{222} + 2.7367. \end{aligned}$$

Remark 7.4. We take $c = 3 > f(0)$ to ensure the Archimedean property, but in the present case the convergence status ξ does not seem to depend on c. Dropping the condition $c - f(\boldsymbol{x}) \geq 0$ in $\tilde{K}$ also leads to an accurate computed optimum.

We obtain the result $\min_{\boldsymbol{x}\in\widetilde{K}} f(\boldsymbol{x}) \approx f(\boldsymbol{x}^*) = 1.060855\ \mathrm{C}^2/\mathrm{m}^4$ at the first GloptiPoly relaxation $d = d_0 = 1$ (with convergence status $\xi = +1$ and for a computation time of 0.8 seconds). The components of the computed minimizer $\mathbf{h}^*$ are (in C/m^2):

$$\begin{aligned} h_{111} = -0.075476,\ h_{112} = -0.426450,\ h_{122} = 0.088998,\ h_{123} = -0.005937, \\ h_{222} = 0.412070,\ h_{223} = -0.308913,\ h_{333} = 0.609783. \end{aligned}$$

By theorem 7.3, the computed cubic tensor $\mathbf{e}^* \in \Sigma_{[\mathbb{O}^-]}$ the closest to $\mathbf{e}_0$ is simply $\mathbf{e}^* = \mathbf{h}^*$. In Voigt notation,

$$[\mathbf{e}^*] = \begin{pmatrix} -0.075476 & 0.088998 & -0.013521 & -0.005937 & -0.300870 & -0.426450 \\ -0.426450 & 0.412070 & 0.0143797 & -0.308913 & -0.005937 & 0.088998 \\ -0.300870 & -0.308913 & 0.609783 & 0.014379 & -0.013521 & -0.005937 \end{pmatrix} \mathrm{C}/\mathrm{m}^2$$

The distance and the relative distance to cubic piezoelectricity are finally

$$\Delta(\mathbf{e}_0, \overline{\Sigma}_{[\mathbb{O}^-]}) \approx \|\mathbf{e}_0 - \mathbf{e}^*\| = 1.214681\,\mathrm{C/m^2}, \qquad \frac{\|\mathbf{e}_0 - \mathbf{e}^*\|}{\|\mathbf{e}_0\|} = 0.684256.$$

The results obtained for the raw piezoelectricity tensors $\mathbf{e}_0^x$ given in the Appendix D for wurzite $\mathrm{Cr}_x\mathrm{Al}_{1-x}\mathrm{N}$, with different chromium concentrations, are summarized in Table 1.

x	$\Delta(\mathbf{E}_0, \overline{\Sigma}_{[\mathbb{O}^-]})$	$\frac{\|\mathbf{e}_0 - \mathbf{e}^*\|}{\|\mathbf{e}_0\|}$	Computation time (s)
0 (AlN)	1.214681	0.684256	0.7
0.035	1.307327	0.715295	0.7
0.07	1.364909	0.729065	0.8
0.10	1.541726	0.785604	0.6
0.13	1.542293	0.758240	1.0
0.16	1.665883	0.793355	0.6
0.19	1.852505	0.813719	0.7
0.225	1.877377	0.781094	1.2
0.255	1.944763	0.752770	0.7

TABLE 1. Results for the raw piezoelectricity tensors of [49] for different Cr-concentrations x (the distance $\Delta(\mathbf{E}_0, \overline{\Sigma}_{[\mathbb{O}^-]}) \approx \|\mathbf{e}_0 - \mathbf{e}^*\|$ is in $\mathrm{C/m^2}$).

Remark 7.5. The computation times are of the same order of magnitude as for the cubic elasticity case. For this quadratic optimization problem (with 7 variables) as well, they are lower than for the 6 variables but degree 3 optimization problem of section 5.

8. Conclusion

Some isotropy strata of tensorial representations of the orthogonal group are explicitly characterized by polynomial covariants. We have taken advantage of this fact to formulate the computation of the distance to these strata as a polynomial optimization problem. We have used the property that the isotropy classes for the representation of SO(3) on the vector space of elasticity tensors are in general semialgebraic. The present work shows the interest of the characterization of the isotropy classes by means of polynomial covariants, rather than by means of invariants. In particular, the covariant characterization of the cubic piezoelectricity symmetry stratum (theorem 7.2), which is the cornerstone of our methodology, is a new result.

We have then recalled Lasserre's method to solve polynomial optimization problems under semialgebraic constraints. Under the so-called Archimedean hypothesis, this approach consists in writing the initial problem as an infinite semidefinite program from which is constructed a sequence of relaxed semidefinite programs that converges to the desired global minimum. We have presented the corresponding algorithm implemented in the freeware GloptiPoly, in particular its stopping criterion.

We have applied this polynomial optimization method to compute the cubic tensor the closest to a raw (measured) constitutive tensor, both in continuum mechanics elasticity and piezoelectricity. We have considered the following examples

- of an elasticity tensor measured by François and coworkers [25] for an aeronautics Nickel-based single crystal superalloy,
- of nine piezoelectricity tensors computed for wurtzite alloys using Density Functional Theory (DFT) and ab-initio simulations, by Manna and coworkers [49].

In both cases, we took advantage of the distance being a coercive polynomial function to adapt the constraints so that they can satisfy the Archimedean condition, in order to ensure the convergence of the method to the desired minimum.

Appendix A. Explicit harmonic decomposition of an elasticity tensor

An elasticity tensor $\mathbf{E} \in \mathbb{E}\mathrm{la}$ admits the following explicit harmonic decomposition [7]:

$$\mathbf{E} = \mathbf{E}^{iso} + \mathbf{q} \underset{(4)}{\otimes} \mathbf{a} + \mathbf{q} \underset{(2,2)}{\otimes} \mathbf{b} + \mathbf{H}. \tag{26}$$

where

$$\mathbf{E}^{iso} = \frac{1}{15}\,(\alpha + 2\beta)\,\mathbf{q} \underset{(4)}{\otimes} \mathbf{q} + \frac{1}{6}\,(\alpha - \beta)\,\mathbf{q} \underset{(2,2)}{\otimes} \mathbf{q}, \tag{27}$$

$$\alpha = \mathrm{tr}(\mathbf{d}), \qquad \beta = \mathrm{tr}(\mathbf{v}), \tag{28}$$

and

$$\mathbf{a} = \frac{2}{7}(\mathbf{d}' + 2\mathbf{v}'), \qquad \mathbf{b} = 2(\mathbf{d}' - \mathbf{v}'). \tag{29}$$

with $\mathbf{d}' = \mathbf{d} - \frac{1}{3}\,\mathrm{tr}(\mathbf{d})\mathbf{q}$ and $\mathbf{v}' = \mathbf{v} - \frac{1}{3}\,\mathrm{tr}(\mathbf{v})\mathbf{q}$ respectively the traceless parts of $\mathbf{d} = \mathrm{tr}_{12}\,\mathbf{E}$ and $\mathbf{v} = \mathrm{tr}_{13}\,\mathbf{E}$.

In (26), $\mathbf{q}$ is the Euclidean canonical bilinear 2-form represented by the components (δ_{ij}) in any orthonormal basis and the tensor products $\underset{(4)}{\otimes}$ and $\underset{(2,2)}{\otimes}$, between symmetric second-order tensors $\mathbf{a}$, $\mathbf{b}$, are defined as follows:

$$(\mathbf{a} \underset{(4)}{\otimes} \mathbf{b})_{ijkl} = (\mathbf{a} \odot \mathbf{b})_{ijkl} = \frac{1}{6}(a_{ij}b_{kl} + b_{ij}a_{kl} + a_{ik}b_{jl} + b_{ik}a_{jl} + a_{il}b_{jk} + b_{il}a_{jk}),$$

and

$$(\mathbf{a} \underset{(2,2)}{\otimes} \mathbf{b})_{ijkl} = \frac{1}{6}(2a_{ij}b_{kl} + 2b_{ij}a_{kl} - a_{ik}b_{jl} - a_{il}b_{jk} - b_{ik}a_{jl} - b_{il}a_{jk}).$$

We have, for Euclidean norm,

$$\|\mathbf{E}\|^2 = 5\alpha^2 + 4\beta^2 + \frac{2}{21}\|\mathbf{d}' + 2\mathbf{v}'\|^2 + \frac{4}{3}\|\mathbf{d}' - \mathbf{v}'\|^2 + \|\mathbf{H}\|^2,$$

Using (28)–(29) we obtain for the experimental elasticity tensor $\mathbf{E}_0$ (given by (15)) the harmonic decomposition

$$\mathbf{E}_0 = (\alpha_0, \beta_0, \mathbf{d}'_0, \mathbf{v}'_0, \mathbf{H}_0)$$

with

$$\alpha_0 = 1531, \qquad \beta_0 = 1479,$$

$$\mathbf{d}'_0 = \begin{pmatrix} \frac{11}{3} & 2 & 14 \\ 2 & \frac{5}{3} & 23 \\ 14 & 23 & -\frac{16}{3} \end{pmatrix} \text{ GPa }, \qquad \mathbf{v}'_0 = \begin{pmatrix} -1 & -11 & -1 \\ -11 & 9 & -1 \\ -1 & -1 & -8 \end{pmatrix} \text{ GPa},$$

$$\mathbf{E}_0^{iso} = \frac{1}{15}\,(\alpha_0 + 2\beta_0)\,\mathbf{q} \underset{(4)}{\otimes} \mathbf{q} + \frac{1}{6}\,(\alpha_0 - \beta_0)\,\mathbf{q} \underset{(2,2)}{\otimes} \mathbf{q},$$

and, in Voigt notation,

$$[\mathbf{H}_0] = \begin{pmatrix} -\frac{1986}{35} & \frac{1093}{35} & \frac{893}{35} & 5 & \frac{352}{7} & -\frac{99}{7} \\ \frac{1093}{35} & -\frac{2306}{35} & \frac{1213}{35} & -31 & \frac{3}{7} & \frac{132}{7} \\ \frac{893}{35} & \frac{1213}{35} & -\frac{2106}{35} & 26 & -\frac{355}{7} & -\frac{33}{7} \\ 5 & -31 & 26 & \frac{1213}{35} & -\frac{33}{7} & \frac{3}{7} \\ \frac{352}{7} & \frac{3}{7} & -\frac{355}{7} & -\frac{33}{7} & \frac{893}{35} & 5 \\ -\frac{99}{7} & \frac{132}{7} & -\frac{33}{7} & \frac{3}{7} & 5 & \frac{1093}{35} \end{pmatrix} \text{ GPa.}$$

Appendix B. Components of second-order covariant $\mathbf{d}_2'$

B.1. **Elasticity tensor case.** The components $(\mathbf{d}_2')_{ij} = (\mathbf{d}_2)_{ij} - \frac{1}{3}(\mathbf{d}_2')_{kk}\delta_{ij}$ of $\mathbf{d}_2 = \mathbf{H} \vdots \mathbf{H}$, with $\mathbf{H}$ the fourth-order harmonic tensor given by (18), are:

$$\begin{aligned}
(\mathbf{d}_2')_{11} &= \frac{2}{3}\big(-4\Lambda_1^2 - \Lambda_1\Lambda_2 - \Lambda_1\Lambda_3 + 2\Lambda_2^2 + 2\Lambda_2\Lambda_3 + 2\Lambda_3^2 + X_1^2 - 4X_1X_2 - 4X_2^2 \\
&\quad + Y_1^2 + 5Y_1Y_2 + 2Y_2^2 - 2Z_1^2 - Z_1Z_2 + 2Z_2^2\big), \\
(\mathbf{d}_2')_{22} &= -\frac{2}{3}\big(-2\Lambda_1^2 + \Lambda_1\Lambda_2 - 2\Lambda_1\Lambda_3 + 4\Lambda_2^2 + \Lambda_2\Lambda_3 - 2\Lambda_3^2 + 2X_1^2 + X_1X_2 - 2X_2^2 \\
&\quad - Y_1^2 + 4Y_1Y_2 + 4Y_2^2 - Z_1^2 - 5Z_1Z_2 - 2Z_2^2\big), \\
(\mathbf{d}_2')_{12} &= 3X_1Y_1 + 3X_2Y_1 - 4X_1Y_2 - X_2Y_2 + 4Z_1\Lambda_1 + Z_2\Lambda_1 + 3Z_1\Lambda_2 - Z_2\Lambda_2 - 2Z_1\Lambda_3, \\
(\mathbf{d}_2')_{13} &= 3X_1(Z_1 + Z_2) - X_2(4Z_1 + Z_2) + 3Y_1\Lambda_1 - Y_2\Lambda_1 - 2Y_1\Lambda_2 + 4Y_1\Lambda_3 + Y_2\Lambda_3, \\
(\mathbf{d}_2')_{23} &= 3Y_1Z_1 + 3Y_2Z_1 - 4Y_1Z_2 - Y_2Z_2 - 2X_1\Lambda_1 + 4X_1\Lambda_2 + X_2\Lambda_2 + 3X_1\Lambda_3 - X_2\Lambda_3.
\end{aligned}$$

B.2. **Piezoelectricity tensor case.** The components $(\mathbf{d}_2')_{ij} = (\mathbf{d}_2)_{ij} - \frac{1}{3}(\mathbf{d}_2')_{kk}\delta_{ij}$ of $\mathbf{d}_2 = \mathbf{h} : \mathbf{h}$ are:

$$\begin{aligned}
(\mathbf{d}_2')_{11} &= \frac{2}{3}\left(h_{111}^2 - 3h_{112}H_{222} - 2h_{222}^2 + 3h_{223}h_{333} + h_{333}^2\right), \\
(\mathbf{d}_2')_{22} &= -\frac{2}{3}\left(2h_{111}^2 + 3h_{111}h_{122} - h_{222}^2 + h_{333}(3h_{223} + 2h_{333})\right), \\
(\mathbf{d}_2')_{12} &= h_{111}(2h_{112} + h_{222}) + 3h_{112}h_{122} + 2h_{122}h_{222} - 2h_{123}h_{333}, \\
(\mathbf{d}_2')_{13} &= h_{111}h_{223} + h_{122}(3h_{223} + h_{333}) - 2h_{123}h_{222}, \\
(\mathbf{d}_2')_{23} &= -2h_{111}h_{123} - h_{112}(3h_{223} + 2h_{333}) - h_{222}(h_{223} + h_{333}).
\end{aligned}$$

Appendix C. Proof of theorem 7.2

Smith and Bao [67] have derived a minimal integrity basis of five invariants for the algebra $\mathbb{R}[\mathbb{H}^3(\mathbb{R}^3)]^{\mathrm{SO}(3)}$, of polynomial SO(3)-invariants of the third-order harmonic tensors $\mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$. These five invariants (equations (2.3) and (2.4) in [67]) can be recast in a more intrinsic form as

$$\begin{gathered}
I_2 = \|\mathbf{h}\|^2, \qquad K_4 = \operatorname{tr} \mathbf{d}_2^2, \qquad I_6 = \|\boldsymbol{v}_3\|^2, \\
K_{10} = \mathbf{h}(\boldsymbol{v}_3, \boldsymbol{v}_3, \boldsymbol{v}_3), \qquad K_{15} = \det(\boldsymbol{v}_3, \mathbf{d}_2 \cdot \boldsymbol{v}_3, \boldsymbol{v}_3 \cdot \mathbf{h} \cdot \boldsymbol{v}_3),
\end{gathered}$$

where $\mathbf{d}_2 = \mathbf{h} : \mathbf{h}$ and $\boldsymbol{v}_3 := \mathbf{h} : \mathbf{d}_2'$. In [59], Olive and Auffray have used these results to deduce that a minimal integrity basis for the algebra $\mathbb{R}[\mathbb{H}^3(\mathbb{R}^3)]^{\mathrm{O}(3)}$, of polynomial O(3)-invariants of $\mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$ consists of the four invariants

$$I_2, \quad K_4, \quad I_6, \quad \text{and} \quad K_{10}.$$

Here, we will formulate alternative integrity bases for both $\mathbb{R}[\mathbb{H}^3(\mathbb{R}^3)]^{\mathrm{SO}(3)}$ and $\mathbb{R}[\mathbb{H}^3(\mathbb{R}^3)]^{\mathrm{O}(3)}$, which happen to be more useful in order to characterize the cubic symmetry class in $\mathbb{H}^3(\mathbb{R}^3)$ for O(3). These will be used to prove theorem 7.2.

Theorem C.1. *Let* $\mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$ *be an harmonic third-order tensor,* $\mathbf{d}_2 = \mathbf{h} : \mathbf{h}$*, and*

$$\boldsymbol{v}_3 := \mathbf{h} : \mathbf{d}_2', \qquad \boldsymbol{v}_5 := \mathbf{d}_2' \cdot \boldsymbol{v}_3, \qquad \boldsymbol{v}_7 := \mathbf{d}_2' \cdot \boldsymbol{v}_5 \quad \textit{where} \quad \mathbf{d}_2' = \mathbf{d}_2 - \frac{1}{3}\operatorname{tr}(\mathbf{d}_2)\mathbf{q}.$$

(1) *A minimal integrity basis of* $\mathbb{R}[\mathbb{H}^3(\mathbb{R}^3)]^{\mathrm{SO}(3)}$ *is constituted by the five invariants*

$$I_2 := \operatorname{tr}\mathbf{d}_2 = \|\mathbf{h}\|^2, \qquad I_4 := \operatorname{tr}(\mathbf{d}_2'^2) = \|\mathbf{d}_2'\|^2, \qquad I_6 := \|\boldsymbol{v}_3\|^2,$$
$$I_{10} := \|\mathbf{d}_2' \times \boldsymbol{v}_3\|^2, \qquad I_{15} := \det(\boldsymbol{v}_3, \boldsymbol{v}_5, \boldsymbol{v}_7).$$

(2) *A minimal integrity basis of* $\mathbb{R}[\mathbb{H}^3(\mathbb{R}^3)]^{\mathrm{O}(3)}$ *is constituted by the four invariants* I_2*,* I_4*,* I_6*, and* I_{10}*.*

Proof. To prove the theorem, it is enough to show that Smith and Bao's invariants can be expressed as polynomials of I_2, I_4, I_6, I_{10}, I_{15}, since, then, this set will be generating and moreover the cardinal of a minimal integrity basis of homogeneous invariants does not depend on the choice of a particular basis [20]. Indeed, one can check that

$$\begin{aligned}
K_4 &= I_4 + \frac{1}{3}{I_2}^2,\\
K_{10} &= -\frac{4}{3}I_{10} - \frac{1}{27}{I_2}^3 I_4 + \frac{1}{9}{I_2}^2 I_6 + \frac{2}{9}I_2{I_4}^2 + \frac{2}{3}I_4 I_6,\\
K_{15} &= 2I_{15},
\end{aligned}$$

which achieves the proof. □

Proof of theorem 7.2. Let $\mathbf{e} = \mathbf{g} + \mathbf{h}$ be a piezoelectricity tensor,

$$\mathbf{g} = (\boldsymbol{v}, \boldsymbol{w}, \mathbf{a}) \in \mathbb{H}^1(\mathbb{R}^3) \oplus \mathbb{H}^1(\mathbb{R}^3) \oplus \mathbb{H}^{2\sharp}(\mathbb{R}^3), \qquad \mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3).$$

If $\mathbf{e} \in \overline{\Sigma}_{[\mathbb{O}^-]}$, then $\mathbf{g} = (\boldsymbol{v}, \boldsymbol{w}, \mathbf{a}) \in \overline{\Sigma}_{[\mathbb{O}^-]}$ vanishes since an element in $\mathbb{H}^1(\mathbb{R}^3)$ or $\mathbb{H}^{2\sharp}(\mathbb{R}^3)$ with at least cubic symmetry ($[\mathbb{O}^-]$) is necessarily isotropic. For the same reason $\mathbf{d}_2'(\mathbf{h}) = 0$. Conversely, if $\mathbf{g} = 0$, then $\mathbf{e} = \mathbf{h} \in \mathbb{H}^3(\mathbb{R}^3)$ is harmonic, and it suffices to show that $\mathbf{h} \in \overline{\Sigma}_{[\mathbb{O}^-]}$ (is at least cubic). Since we assume furthermore $\mathbf{d}_2' = 0$, we have

$$I_2(\mathbf{h}) = \|\mathbf{h}\|^2 \geq 0, \qquad I_4(\mathbf{h}) = 0, \qquad I_6(\mathbf{h}) = 0, \qquad I_{10}(\mathbf{h}) = 0.$$

Now an harmonic tensor in $\mathbb{H}^3(\mathbb{R}^3)$ which is fixed by $\mathbb{O}^-$ is written (in Voigt notation (24)) as

$$\mathbf{h}_0 = \delta \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

For such a tensor we get

$$I_2(\mathbf{h}_0) = 6\delta^2, \qquad I_4(\mathbf{h}_0) = 0, \qquad I_6(\mathbf{h}_0) = 0, \qquad I_{10}(\mathbf{h}_0) = 0.$$

Therefore, since $I_2(\mathbf{h}) = \|\mathbf{h}\|^2 \geq 0$, we can find a real number δ such that $6\delta^2 = I_2(\mathbf{h})$, and thus an at least cubic tensor $\mathbf{h}_0$ such that

$$I_2(\mathbf{h}_0) = I_2(\mathbf{h}), \qquad I_4(\mathbf{h}_0) = I_4(\mathbf{h}), \qquad I_6(\mathbf{h}_0) = I_6(\mathbf{h}), \qquad I_{10}(\mathbf{h}_0) = I_{10}(\mathbf{h}).$$

But an integrity basis for a real representation of a compact group *separate the orbits* [2, Appendix C]. Hence, $\mathbf{h}$ and $\mathbf{h}_0$ are necessarily in the same orbit, which means that $\mathbf{h} = \rho_3(g)\mathbf{h}_0$, for some $g \in \mathrm{O}(3)$. □

Appendix D. Raw piezoelectricity tensors for wurtzite

The raw piezoelectricity tensors $\mathbf{e}_0^x$ considered in section 7 correspond to the mean values computed in [49] for wurtzite $\mathrm{Cr}_x\mathrm{Al}_{1-x}\mathrm{N}$, with x the chromium concentration (in $\mathrm{C/m^2}$),

$$[\mathbf{e}_0^{0.035}] = \begin{pmatrix} -0.0329 & 0.0599 & -0.0195 & 0.0267 & -0.2327 & -0.0988 \\ -0.0548 & -0.0129 & -0.0063 & -0.2075 & -0.0051 & -0.0293 \\ -0.5872 & -0.4900 & 1.5560 & -0.0218 & -0.0278 & -0.0115 \end{pmatrix},$$

$$[\mathbf{e}_0^{0.07}] = \begin{pmatrix} -0.0393 & 0.0185 & 0.0048 & 0.0290 & -0.2171 & -0.0436 \\ -0.07 & 0.0554 & 0.0137 & -0.1574 & 0.0198 & 0.0044 \\ -0.5179 & -0.5886 & 1.6521 & -0.0085 & -0.0095 & -0.0119 \end{pmatrix},$$

$$[\mathbf{e}_0^{0.10}] = \begin{pmatrix} 0.0291 & -0.0141 & -0.0523 & -0.0016 & 0.0028 & 0.0138 \\ -0.0611 & 0.0819 & -0.0567 & -0.1841 & 0.0116 & 0.0270 \\ -0.5244 & -0.5918 & 1.7715 & -0.0018 & 0.0066 & -0.0145 \end{pmatrix},$$

$$[\mathbf{e}_0^{0.13}] = \begin{pmatrix} -0.0985 & 0.1138 & 0.047 & -0.0169 & -0.0169 & -0.0984 \\ 0.0558 & 0.0183 & -0.0367 & -0.1735 & -0.0384 & 0.0474 \\ -0.5441 & -0.5455 & 1.8506 & -0.0148 & -0.0016 & -0.0193 \end{pmatrix},$$

$$[\mathbf{e}_0^{0.16}] = \begin{pmatrix} 0.0315 & -0.0375 & 0.0273 & 0.0206 & 0.0206 & 0.0933 \\ -0.215 & -0.0717 & 0.0845 & -0.2157 & 0.0438 & -0.0332 \\ -0.4517 & -0.5587 & 1.9243 & 0.0447 & 0.0277 & -0.0482 \end{pmatrix},$$

$$[\mathbf{e}_0^{0.19}] = \begin{pmatrix} 0.4524 & 0.3564 & -0.0827 & -0.0276 & -0.0276 & 0.1067 \\ -0.0783 & 0.0868 & 0.0318 & 0.0037 & -0.1053 & -0.0765 \\ -0.5768 & -0.4566 & 2.0350 & -0.1332 & -0.1016 & -0.1253 \end{pmatrix},$$

$$[\mathbf{e}_0^{0.225}] = \begin{pmatrix} 0.0428 & 0.0974 & -0.0429 & -0.0319 & -0.0363 & 0.0099 \\ -0.1399 & -0.2386 & -0.0253 & -0.1505 & 0.0143 & -0.1770 \\ -0.5800 & -0.5552 & 2.2197 & 0.0164 & 0.0048 & 0.0234 \end{pmatrix},$$

$$[\mathbf{e}_0^{0.255}] = \begin{pmatrix} -0.0914 & 0.0758 & 0.0000 & -0.0022 & -0.2835 & 0.0000 \\ 0.0000 & -0.0022 & 0.0000 & -0.2660 & 0.0002 & -0.0020 \\ -0.6063 & -0.5847 & 2.3709 & -0.0714 & -0.0738 & -0.0559 \end{pmatrix}.$$

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Chapter 6

Distance to isotropy strata by Euler Lagrange method

This chapter is an ArXiv preprint [4] in which we solve the same problem of the distance to isotropy strata introduced in the previous chapter but here using an analytic method for solving polynomial optimization problems based on Euler-Lagrange equations. Euler-Lagrange method for solving constrained polynomial optimization problems, consists in formulating the constrained problem to an unconstrained one with the help of Lagrange multipliers. This comes down to find the critical points of a polynomial function leading to a system of polynomial equations that can be solved using Gröbner basis (for example). With this method, we were able to solve the problem for some numerical examples, first in cubic elasticity and then in cubic elasto-plasticity for instance. However, a submersion condition is imposed on the constraints functions in order to apply this method which restrict the possible cases for which this method can be applied. For instance, finding the closest cubic piezoelectricity tensor to an experimental one, which has been already done for some examples using Lasserre's method in section 7 of the previous chapter, cannot be done using Euler-Lagrange method since the Jacobian of the constraint function does not have maximal rank and so the submersion condition is not satisfied.

THE DISTANCE TO CUBIC SYMMETRY CLASS AS A POLYNOMIAL OPTIMIZATION PROBLEM

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Abstract. Generically, a fully measured elasticity tensor has no material symmetry. For single crystals with a cubic lattice, or for the aeronautics turbine blades superalloys such as Nickel-based CMSX-4, cubic symmetry is nevertheless expected. It is in practice necessary to compute the nearest cubic elasticity tensor to a given raw one. Mathematically formulated, the problem consists in finding the distance between a given tensor and the cubic symmetry stratum.

It is known that closed symmetry strata (for any tensorial representation of the rotation group) are semialgebraic sets, defined by polynomial equations and inequalities. It has been recently shown that the closed cubic elasticity stratum is moreover algebraic, which means that it can be defined by polynomial equations only (without requirement to polynomial inequalities). We propose to make use of this mathematical property to formulate the distance to cubic symmetry problem as a polynomial (in fact quadratic) optimization problem, and to derive its quasi-analytical solution using the technique of Gröbner bases. The proposed methodology also applies to cubic Hill elasto-plasticity (where two fourth-order constitutive tensors are involved).

1. Introduction

Anisotropic elasto-plasticity theories introduce (at least) two fourth-order constitutive tensors, the Hooke and the Hill tensors for instance. It is nowadays possible to measure/determine all their components [41, 8, 7, 27, 29, 16, 29, 46]. These measured constitutive tensors are however generically triclinic (they have no material symmetry).

On the other hand, many materials (such as composite/engineered materials, single crystal superalloys or rocks) have an expected symmetry, most often due to their microstructure and their elaboration process. In practice, appealing to Curie principle ("the symmetries of the causes are to be found in the effects"), their constitutive tensors shall inherit the material symmetry (orthotropy, cubic or monoclinic symmetry for example), so that the natural question is *to determine the constitutive tensor with a given material symmetry the nearest to a given measured (triclinic) constitutive tensor.* This question has been extensively studied, from both the theoretical and numerical points of view, since the pioneering work of Gazis, Tadjbakhsh and Toupin [31], and subsequent works in the 90s [8, 7, 27, 22, 29]. Most works focus on the elasticity tensor [31, 25, 27, 28, 34, 22, 29, 21, 47, 40, 24, 48], a few ones on the piezoelectricity tensor [66]. So far, we are not aware of some similar studies for the Hill plasticity tensor or the combination of several constitutive tensors.

Even if some analytical attempts exist [31, 63, 59, 6], the *distance to an elasticity symmetry class problem* is usually solved numerically, following [27, 29, 22, 21], using the parameterization of a symmetry class, by its normal form $\mathbf{A}$ (for instance (8) for cubic symmetry [25]) and a rotation Q,

$$\mathbf{E} = Q \star \mathbf{A} \quad \text{with components} \quad E_{ijkl} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}A_{pqrs}$$

where $\star$ stands for the action of the rotation Q on the tensor $\mathbf{A}$ [26, 63]. Letting $\mathbf{E}_0$ be the given experimental (raw) elasticity tensor, one has thus to solve the minimization problem

$$\min_{Q,\,\mathbf{A}} \|\mathbf{E}_0 - Q \star \mathbf{A}\|^2. \tag{1}$$

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The rotation Q can be parameterized by the Euler angles or by a unit quaternion q [21, 39, 40], allowing, in the second case, for the formulation of the considered distance problem as a *polynomial optimization problem*. Indeed, the function $\|\mathbf{E}_0 - Q(\mathrm{q}) \star \mathbf{A}\|^2$ is then quadratic in $\mathbf{A}$ and polynomial of degree 16 in q. Note, however, that a pair $(Q, \mathbf{A})$ is far from representing uniquely a tensor $\mathbf{E}$. For instance, a cubic elasticity tensor $\mathbf{E}$ is represented by 24 pairs $(Q, \mathbf{A})$ or 48 pairs $(\mathrm{q}, \mathbf{A})$ (since $Q(\mathrm{q}) = Q(-\mathrm{q})$). This means that we expect to find at least 24 global minima $(Q, \mathbf{A})$, or 48 global minima $(\mathrm{q}, \mathbf{A})$ to problem (1), which correspond to the same cubic elasticity tensor $\mathbf{E}$. More generally, there are at least as many global minima $(Q, \mathbf{A})$ as there are symmetries of $\mathbf{A}$ (24 for cubic symmetry).

Since the variables Q and $\mathbf{A}$ are independent, if G is the symmetry group of the considered material, the minimum (1) can be rewritten as [29]

$$\min_{Q} \|\mathbf{E}_0 - Q \star \mathbf{R}_G(Q^T \star \mathbf{E}_0)\|^2, \tag{2}$$

where $\mathbf{R}_G$ is the Reynolds operators [60, Chapter 2] (orthogonal projector of $\mathbb{E}\mathrm{la}$ onto the vector space $\operatorname{Fix} G$ of considered normal forms $\mathbf{A}$) and, here for finite groups, defined explicitly by

$$\mathbf{R}_G(\mathbf{C}) := \frac{1}{|G|} \sum_{R \in G} R \star \mathbf{C},$$

where $|G|$ is the order of the group G. Definition (2) is the expression of the distance to a symmetry class adopted by most authors. It has the advantage of removing one variable $\mathbf{A}$ in the minimization problem but the disadvantage of doubling the degree in Q and thus in q.

Solving the distance to a given symmetry problem (1) is usually done numerically with, then, the risk to reach a local minimum instead of a global one [29, 47, 20]. To overcome this difficulty, François and coworkers proposed to plot first pole figures for the given elasticity tensor $\mathbf{E}_0$ [27, 28] (renamed plots of the monoclinic distance in [47, 40]). Accordingly, they got an initial value for $\mathbf{E}$, not too far from $\mathbf{E}_0$, which was then optimized by a standard numerical (iterative) scheme.

Computational algebraic or semialgebraic optimization methods have been developed to find (directly) the global minimum of a multi-variable polynomial function (with polynomial constraints), using semidefinite programming for example [50, 5, 62, 61, 44, 65, 43]. On the other hand, there are nowadays symbolic computation methods to solve sets of polynomial equations, for instance the method of Gröbner bases [17] (see also [19, 60]). These methods work well when the number of variables (*i.e.*, of unknowns) is small and when the degree of the polynomials remains low [43]. The Gröbner basis method is available in the algebraic geometry software Macaulay2 [32] and in most Computer Algebra Systems. It does not make any numerical approximation if the coefficients of the considered polynomials are rational numbers and the Gröbner basis method can be seen as quasi-analytical. We use the prefix *quasi* because at one step, after an exact variables elimination process, one has to solve a polynomial equation in one variable, the remaining equations becoming afterwards linear.

The elasticity symmetry classes have been characterized by polynomial equations and inequalities in [53] (see also [2], or [9] for the case of harmonic fourth-order tensors), illustrating the mathematical property that the closed SO(3)-symmetry strata[1] are semialgebraic sets [3, 4, 55, 57]. The necessary and sufficient conditions for a Hooke tensor to belong to one of the eight elasticity symmetry strata have been formulated using polynomial covariants (in a coordinate-free manner). For a Hooke tensor, the cubic stratum is characterized by quadratic equations [53, Theorem 10.3]. Therefore, one hopes to formulate the *distance to cubic elasticity problem* as a quadratic optimization problem (of much lower degree than for the normal form/quaternion parameterization method) and expects a quasi-analytical solution using the Gröbner basis method. To succeed, one will simply have to derive first-order Euler–Lagrange equations for the corresponding quadratic optimization problem.

Cubic symmetry is of most importance for Ni-based single crystal superalloys, such as CMSX-4 [30, 54, 56], the material of aircrafts gas turbine blades (subject to (visco-)plasticity [45, 13]). Thanks to the harmonic decomposition [10, 58, 18, 11], the geometry of cubic fourth order

[1] A symmetry stratum is the set of all tensors which have the same symmetry class.

tensors is now well understood. This will make it possible to formulate the calculation of the distance to cubic symmetry as a polynomial optimization problem, not only for a single elasticity tensor, but also for a pair $(\mathbf{E}, \mathbf{P})$ of two fourth-order constitutive tensors. Here, $\mathbf{E}$ is understood as the Hooke (elasticity) tensor and $\mathbf{P}$ as the Hill (plasticity) tensor. Indeed, we shall see that this pair of tensors is at least cubic if and only if the harmonic second-order components of $\mathbf{E}$ and $\mathbf{P}$ vanish and if their harmonic fourth-order components are at least cubic and proportional.

We will make use of the reformulation of the *distance to cubic elasticity* as a *quadratic optimization problem*, in order to solve it quasi-analytically. In practice, this will be done thanks to the *theory of Gröbner bases*. We will take advantage of the fact that the material parameters, such as the components of an experimental elasticity tensor, are measured with only a few significant digits to work with rational coefficients polynomials. This point is of main importance in the resolution of a system of polynomial equations by the obtention of a Gröbner basis (see remark A.1 in the Appendix).

The paper is organized as follows. The Euler–Lagrange method for solving constrained optimization problems is briefly presented in section 2. Background materials on cubic constitutive tensors are recalled in section 3 and section 4. The problem of the distance to cubic elasticity is formulated as a polynomial (quadratic) optimization problem in section 5 and solved thanks to the theory of Gröbner bases in section 6. The extension to the pair $(\mathbf{E}, \mathbf{P})$ of the Hooke and Hill tensors is described in section 7 and section 8. Finally, in section 9, we explain how to compute a natural cubic basis for any given cubic Hooke tensor. To be self-contained, a summary of Gröbner bases methods for algebraic elimination is provided in Appendix A. Last, the lack of accuracy of some upper bounds estimates of the distance to cubic elasticity is discussed in Appendix B.

Notations. We are working in orthonormal bases, so that we do not have to distinguish between covariant and contravariant tensors. The tensor product is denoted by $\otimes$. An *harmonic tensor* is a traceless totally symmetric tensor. The space of harmonic tensors of order n will be denoted by $\mathbb{H}^n(\mathbb{R}^3)$ or simply $\mathbb{H}^n$. It is a subspace of dimension $2n+1$ of the vector space $\mathbb{S}^n(\mathbb{R}^3)$, the space of totally symmetric tensors $\mathbf{S} = \mathbf{S}^s$ of order n (where $(\cdot)^s$ is the symmetrization operator).

Let $\mathbf{S} = \mathbf{S}^s \in \mathbb{S}^p(\mathbb{R}^3)$ (of order p) and $\mathbf{T} = \mathbf{T}^s \in \mathbb{S}^q(\mathbb{R}^3)$ (of order q) be two totally symmetric tensors. The *totally symmetric tensor product* $\odot$ is defined by

$$\mathbf{S} \odot \mathbf{T} := (\mathbf{S} \otimes \mathbf{T})^s \in \mathbb{S}^{p+q}(\mathbb{R}^3).$$

It is a totally symmetric tensor (of order $p+q$). The *generalized cross product* between two totally symmetric tensors, which was introduced in [53], is defined by

$$\mathbf{S} \times \mathbf{T} := (\mathbf{T} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{S})^s \in \mathbb{S}^{p+q-1}, \tag{3}$$

where $\boldsymbol{\varepsilon} = (\varepsilon_{ijk})$ is the Levi-Civita tensor. In components, it is written as

$$(T_{i_1 \dots i_{p-1} k}\, \varepsilon_{k i_p l}\, S_{l i_{p+1} \dots i_{p+q-1}})^s.$$

A dot denotes a contraction between two tensors and several dots, several contractions. For instance

$$(\mathbf{a} \cdot \mathbf{b})_{ij} = a_{ik} b_{kj}, \qquad \mathbf{a} : \mathbf{b} = a_{ij} b_{ij},$$

$$(\mathbf{H} : \mathbf{a})_{ij} = H_{ijkl} a_{kl}, \qquad (\mathbf{H} : \mathbf{K})_{ijkl} = H_{ijpq} K_{pqkl}, \qquad (\mathbf{H} \vdots \mathbf{K})_{ij} = H_{ipqr} K_{pqrj},$$

where $\mathbf{a}$, $\mathbf{b}$ are second-order tensors and $\mathbf{H}$, $\mathbf{K}$, fourth-order tensors. The usual abbreviations $\mathbf{H}^2 = \mathbf{H} : \mathbf{H}$ and $\mathbf{H}^3 = \mathbf{H} : \mathbf{H} : \mathbf{H}$ shall also be used.

2. The Euler–Lagrange method for polynomial functions and constraints

The simplest method to solve a minimization problem for a polynomial function f, defined on $\mathbb{R}^n$, is probably the *Euler–Lagrange method*, which consists in looking for its critical points. The critical points of f are solutions of a system of algebraic equations which may be solved

using *Gröbner bases* for example (see Appendix A). When, moreover, polynomial algebraic constraints $g(\boldsymbol{x}) = 0$ are involved, where

$$g : \mathbb{R}^n \to \mathbb{R}^p,$$

is a smooth vector-valued function, the *method of Lagrange multipliers* can be used [12, 38, 42]. In geometric terms, the constraint problem means that we seek for critical points of the restriction of f to the submanifold of $\mathbb{R}^n$

$$S := \{\boldsymbol{x} \in \mathbb{R}^n;\ g(\boldsymbol{x}) = 0\}\,. \tag{4}$$

This requires that the constraint function, $g : \mathbb{R}^n \to \mathbb{R}^p$, is a *submersion* on $S = g^{-1}(0)$, which means that the linear tangent map (*i.e.*, here the Jacobian matrix)

$$T_{\boldsymbol{x}} g : \mathbb{R}^n \to \mathbb{R}^p$$

is of maximal rank p at each point $\boldsymbol{x} \in S$ (which requires that $n \geq p$). This condition ensures that S is a smooth *submanifold* of $\mathbb{R}^n$ of dimension $n - p$ [42]. In that case, one can show, using the implicit function theorem, that the solutions of the constrained problem

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{with} \quad g(\boldsymbol{x}) = 0, \tag{5}$$

are critical points of the function

$$F(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + (\boldsymbol{\lambda}, g(\boldsymbol{x})), \tag{6}$$

where $(\cdot, \cdot)$ is the duality bracket on $\mathbb{R}^p$ and the dual variable $\boldsymbol{\lambda}$ is the *Lagrange multiplier*. A proof of this fact can be found in [1, Theorem 3.5.27].

Remark 2.1. Note however that the extrema of f are in general saddle points of F [38]. Therefore, one should not make the false statement that the minimization of the constrained problem (5) is equivalent to the minimization of the function (6).

The critical points of (6) are the solutions of the algebraic system

$$\begin{cases} \dfrac{\partial F}{\partial \boldsymbol{x}} = \dfrac{\partial f}{\partial \boldsymbol{x}} + \left(\boldsymbol{\lambda}, \dfrac{\partial g}{\partial \boldsymbol{x}}\right) = 0, \\ \dfrac{\partial F}{\partial \boldsymbol{\lambda}} = g = 0. \end{cases} \tag{7}$$

These equations are referred to as (first-order) *Euler–Lagrange equations with constraints.*

In practice, however, the problem is not that simple. In several problems, the set $S = g^{-1}(0)$ contains some point $\boldsymbol{x}$ at which g is not a submersion. Worse, in the following example, which concerns the distance of a deviatoric second order tensors $\boldsymbol{x} = \mathbf{h} \in \mathbb{H}^2$ to transverse isotropy, the gradient of g is singular at each point $\mathbf{h}$ of S.

Example 2.2 (The transversely isotropic (closed) strata in $\mathbb{H}^2$)**.** It is the vector subspace S of $\mathbb{H}^2$ of deviatoric tensors which have at least two identical eigenvalues. The set S is defined implicitly by the polynomial equation

$$g(\mathbf{h}) := \left(\operatorname{tr} \mathbf{h}^2\right)^3 - 6\left(\operatorname{tr} \mathbf{h}^3\right)^2 = 0, \qquad \mathbf{h} \in \mathbb{H}^2.$$

Unfortunately, the gradient of g in $\mathbb{H}^2$

$$\operatorname{grad}_{\mathbf{h}} g = 6\left((\operatorname{tr} \mathbf{h}^2)^2 \mathbf{h} - 6(\operatorname{tr} \mathbf{h}^3)(\mathbf{h}^2)'\right)$$

vanishes identically on the set $S = g^{-1}(0)$, since, when $\mathbf{h} \in \mathbb{H}^2$ is transversely isotropic, we have

$$(\mathbf{h}^2)' = \frac{\operatorname{tr} \mathbf{h}^3}{\operatorname{tr} \mathbf{h}^2}\, \mathbf{h}$$

and thus

$$\operatorname{grad}_{\mathbf{h}} g = \frac{6g(\mathbf{h})}{\operatorname{tr} \mathbf{h}^2} \mathbf{h} = 0.$$

Fortunately, all situations are not as bad as in this example but singularities may still exist. In the following examples, concerning respectively cubic fourth-order harmonic tensors and elasticity tensors, of main interest for the present work, the set S is defined by a mapping g which is a submersion on a big open subset of S, but not on all of S.

Example 2.3 (The cubic (closed) strata in $\mathbb{H}^4$)**.** It is the vector subspace S of $\mathbb{H}^4$ of fourth-order harmonic tensors which are at least cubic. It was shown in [53, Theorem 9.3], that this set can be defined as

$$S = \left\{\mathbf{H} \in \mathbb{H}^4;\ g(\mathbf{H}) = 0\right\},$$

where

$$g : \mathbb{H}^4 \to \mathbb{H}^2$$

is a polynomial mapping of degree 2. One can check that g is a submersion at each cubic tensor $\mathbf{H} \neq 0$, but not at $\mathbf{H} = 0$, which is a singular point.

Example 2.4 (The cubic (closed) strata in $\mathbb{E}\mathrm{la}$)**.** It is the vector subspace S of $\mathbb{E}\mathrm{la}$ of elasticity tensors which are at least cubic. It was shown in [53, Theorem 10.2], that this set can be defined as

$$S = \{\mathbf{E} \in \mathbb{E}\mathrm{la};\ g(\mathbf{E}) = 0\},$$

where

$$g : \mathbb{E}\mathrm{la} \to \mathbb{H}^2 \oplus \mathbb{H}^2 \oplus \mathbb{H}^2$$

is a polynomial mapping. One can check that g is a submersion at each point $\mathbf{E} \in S$ if $\mathbf{E}$ is cubic, but not if $\mathbf{E}$ is isotropic.

Remark 2.5. In [33] and [64] are proposed some algorithms to solve the constrained problem (5) even when the polynomial mapping g is not a submersion, under some further hypotheses (the implementation of the algorithm proposed in [33] is available on the webpage of the first author as a Maple library). These algorithms involve the notions of *nonsingular* and *singular* points of the real algebraic set $S = \{\boldsymbol{x} \in \mathbb{R}^n;\ g(\boldsymbol{x}) = 0\}$. Under some hypotheses on S and on the polynomial coordinate functions $(g_1, \ldots, g_p)$ of g, a point $\boldsymbol{x}$ of S is said to be nonsingular if the Jacobian matrix of g at $\boldsymbol{x}$ is of rank $n - d$, where d is the *dimension* of the real algebraic set S (which is by definition the so-called *Krull dimension* of the ring of polynomial functions on S), otherwise $\boldsymbol{x}$ is said to be singular. If the real algebraic set S has no singular point, it is said to be nonsingular and, in this case, S is a smooth submanifold of $\mathbb{R}^n$ of dimension d (precise definitions and properties can be found in [14]). However, the correctness of the subroutine *GenCritValues* of [64, Section 4] is, as far as we understand, not clear for us since it refers to an algorithm of [37] which is carried out on *complex* algebraic sets, not on real ones.

3. Cubic elasticity tensors

The space of elasticity tensors [26], denoted by $\mathbb{E}\mathrm{la}$, is the space of fourth-order tensors $\mathbf{E}$ with the following index symmetries

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}.$$

$\mathbb{E}\mathrm{la}$ is a vector space of dimension 21 and an elasticity tensor $\mathbf{E} \in \mathbb{E}\mathrm{la}$ can be represented in Voigt notation by the matrix

$$[\mathbf{E}] = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & E_{1123} & E_{1113} & E_{1112} \\ E_{1122} & E_{2222} & E_{2233} & E_{2223} & E_{1223} & E_{1222} \\ E_{1133} & E_{2233} & E_{3333} & E_{2333} & E_{1333} & E_{1233} \\ E_{1123} & E_{2223} & E_{2333} & E_{2323} & E_{2331} & E_{2312} \\ E_{1113} & E_{1223} & E_{1333} & E_{2331} & E_{1313} & E_{3112} \\ E_{1112} & E_{1222} & E_{1233} & E_{2312} & E_{3112} & E_{1212} \end{pmatrix}.$$

If $\mathbf{E}$ has *at least* the cubic symmetry, there exists an orthonormal basis $(\boldsymbol{e}_i)$ (called the natural basis or the cubic basis), in which $\mathbf{E}$ has the so-called *cubic normal form* in Voigt representation

$$[\mathbf{E}] = \begin{pmatrix} E_{1111} & E_{1122} & E_{1122} & 0 & 0 & 0 \\ E_{1122} & E_{1111} & E_{1122} & 0 & 0 & 0 \\ E_{1122} & E_{1122} & E_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1212} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}_{(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)} . \tag{8}$$

If $E_{1111} - E_{1122} - 2E_{1212} = 0$, then $\mathbf{E}$ is isotropic. Otherwise, it is cubic. One may point out the cubic symmetry group $(\mathbb{O})$ and write $\mathbf{E}_{\mathbb{O}}$ for the normal form of a cubic tensor $\mathbf{E}$.

If E, ν and G, respectively denote the Young modulus, the Poisson ratio, and the shear modulus of a material, the engineer's expressions for the E_{ijkl} are

$$\begin{cases} E_{1111} = \dfrac{(1-\nu)E}{1-\nu-2\nu^2}, \\ E_{1122} = \dfrac{\nu E}{1-\nu-2\nu^2}, \\ E_{1212} = G, \end{cases}$$

and $G \neq E/2(1+\nu)$ when $\mathbf{E}$ is cubic. In intrinsic notations, a cubic elasticity tensor $\mathbf{E}$ can be rewritten as in [26]

$$\mathbf{E} = 2\mu\,\mathbf{I} + \lambda \mathbf{1} \otimes \mathbf{1} + \mathbf{H}, \qquad \mathbf{H} \neq 0, \tag{9}$$

where $\mathbf{I}$ is the fourth order tensor with components $I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ and $\mathbf{H} \in \mathbb{H}^4$ is a cubic fourth-order harmonic tensor[2]. Here,

$$\lambda = \frac{1}{15}(2\,\mathrm{tr}(\mathrm{tr}_{12}\,\mathbf{E}) - \mathrm{tr}(\mathrm{tr}_{13}\,\mathbf{E})) = \frac{1}{5}(E_{1111} - 2E_{1212} + 4E_{1122}),$$

and

$$\mu = \frac{1}{30}(-\,\mathrm{tr}(\mathrm{tr}_{12}\,\mathbf{E}) + 3\,\mathrm{tr}(\mathrm{tr}_{13}\,\mathbf{E})) = \frac{1}{5}(E_{1111} + 3E_{1212} - E_{1122}),$$

are the Lamé constants.

A fourth-order harmonic tensor has 9 independent components. It can always be parameterized as (in Voigt notation, see [23, 52]),

$$[\mathbf{H}] = \begin{pmatrix} \Lambda_2+\Lambda_3 & -\Lambda_3 & -\Lambda_2 & -X_1 & Y_1+Y_2 & -Z_2 \\ -\Lambda_3 & \Lambda_3+\Lambda_1 & -\Lambda_1 & -X_2 & -Y_1 & Z_1+Z_2 \\ -\Lambda_2 & -\Lambda_1 & \Lambda_1+\Lambda_2 & X_1+X_2 & -Y_2 & -Z_1 \\ -X_1 & -X_2 & X_1+X_2 & -\Lambda_1 & -Z_1 & -Y_1 \\ Y_1+Y_2 & -Y_1 & -Y_2 & -Z_1 & -\Lambda_2 & -X_1 \\ -Z_2 & Z_1+Z_2 & -Z_1 & -Y_1 & -X_1 & -\Lambda_3 \end{pmatrix}. \tag{10}$$

If $\mathbf{H}$ has *at least* the cubic symmetry, there exists an orthonormal basis $(\boldsymbol{e}_i)$, in which (in Voigt notation, see [9]):

$$[\mathbf{H}] = \delta \begin{pmatrix} 8 & -4 & -4 & 0 & 0 & 0 \\ -4 & 8 & -4 & 0 & 0 & 0 \\ -4 & -4 & 8 & 0 & 0 & 0 \\ 0 & 0 & 0 & -4 & 0 & 0 \\ 0 & 0 & 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & 0 & 0 & -4 \end{pmatrix}_{(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)}, \qquad \delta = \frac{1}{4}(\mu - G), \tag{11}$$

with $\delta = 0$ when $\mathbf{H}$ is isotropic and $\delta \neq 0$ when it is cubic.

Remark 3.1. The decomposition (9) of $\mathbf{E}$ into λ, μ, and $\mathbf{H}$ (with $\mathbf{H}$ cubic), is the so-called harmonic decomposition of a cubic elasticity tensor (see [10, 18]).

[2] *i.e.* totally symmetric, $\mathbf{H} = \mathbf{H}^s$, and traceless, $\mathrm{tr}_{ij}\,\mathbf{H} = 0$.

The generalized Lamé constants $\lambda = \lambda(\mathbf{E}), \mu = \mu(\mathbf{E})$ are two (linear) invariants of $\mathbf{E}$. The scalar $\delta = \delta(\mathbf{E})$ is a (rational) invariant of the cubic elasticity tensor $\mathbf{E}$. Indeed, one has then [9, Section 5.1]:

$$\delta = \frac{J_3}{4J_2}, \tag{12}$$

where

$$J_2 = \|\mathbf{H}\|^2 = \operatorname{tr}(\operatorname{tr}_{13}\mathbf{H}^2) = H_{ijkl}H_{ijkl}, \quad \text{and} \quad J_3 = \operatorname{tr}(\operatorname{tr}_{13}\mathbf{H}^3) = H_{ijkl}H_{klpq}H_{pqij}, \tag{13}$$

are two polynomial invariants of $\mathbf{H}$ (first introduced in [15]). The Euclidean squared norm of the cubic elasticity tensor $\mathbf{E}$ is then

$$\|\mathbf{E}\|^2 = 3\left(3\lambda^2 + 4\lambda\mu + 8\mu^2\right) + 480\delta^2.$$

When evaluated on (10), the invariants J_2 and J_3 can be expressed as

$$\begin{aligned} J_2 = 2\Big(&4\Lambda_1^2 + \Lambda_1\Lambda_2 + \Lambda_1\Lambda_3 + 4\Lambda_2^2 + \Lambda_2\Lambda_3 + 4\Lambda_3^2 + 8X_1^2 + 4X_1X_2 + 4X_2^2 \\ &+ 8Y_1^2 + 4Y_1Y_2 + 4Y_2^2 + 8Z_1^2 + 4Z_1Z_2 + 4Z_2^2\Big), \end{aligned} \tag{14}$$

$$\begin{aligned} J_3 = 6\Big(&\Lambda_1^2\Lambda_2 + \Lambda_1\Lambda_2^2 + \Lambda_3^2(\Lambda_1 + \Lambda_2) - 3X_1^2(\Lambda_1 + \Lambda_3) - 2\Lambda_3X_1X_2 \\ &+ 4X_1(\Lambda_2X_2 + (Y_1 + Y_2)(Z_1 + Z_2)) + X_2^2(\Lambda_2 + \Lambda_3) + 4X_2(Z_1(Y_1 + Y_2) + Y_1Z_2) \\ &- 3\Lambda_1Y_1^2 - 3\Lambda_2Y_1^2 + \Lambda_3\left(\Lambda_1^2 - \Lambda_1\Lambda_2 + \Lambda_2^2 + 4Y_1Y_2 + Y_2^2 - 3Z_1^2\right) - 2\Lambda_1Y_1Y_2 \\ &+ \Lambda_1Y_2^2 - 3\Lambda_2Z_1^2 + 4\Lambda_1Z_1Z_2 - 2\Lambda_2Z_1Z_2 + \Lambda_1Z_2^2 + \Lambda_2Z_2^2\Big). \end{aligned} \tag{15}$$

Remark 3.2. Given a cubic elasticity tensor $\mathbf{E}^* = (E^*_{ijkl})$, expressed in an arbitrary basis, the calculation of its normal form $\mathbf{E} = \mathbf{E}_{\mathbb{O}}$ (of Voigt representation (8)) is straightforward (using (11) within (9)). Indeed, the normal form (8) is recovered from the calculation of λ, μ and $\delta = J_3/4J_2$ by the above formulas with

$$E_{1111} = 2\mu + \lambda + 8\delta, \qquad E_{1122} = \lambda - 4\delta, \qquad E_{1212} = \mu - 4\delta, \tag{16}$$

where the invariants λ, μ, J_2, J_3 and δ are evaluated on $\mathbf{E}^*$.

The covariant characterization of the elasticity symmetry classes by polynomial equations (and inequalities) has been performed recently, in [53, theorem 10.2]. The case of the cubic symmetry is recalled as theorem 3.3 below. We denote by

$$\mathbf{a}' = \mathbf{a} - \frac{1}{3}\operatorname{tr}(\mathbf{a})\,\mathbf{1},$$

the deviatoric part of a second-order tensor $\mathbf{a}$, and by $\mathbf{E}^s$, the totally symmetric part of $\mathbf{E}$, with components

$$E^s_{ijkl} = \frac{1}{3}(E_{ijkl} + E_{ikjl} + E_{iljk}).$$

Theorem 3.3 (Olive et al (2021))**.** *Let* $\mathbf{E}$ *be an elasticity tensor,*

$$\mathbf{d} = \operatorname{tr}_{12}\mathbf{E} \quad \textit{and} \quad \mathbf{v} = \operatorname{tr}_{13}\mathbf{E},$$

respectively, the dilatation and the Voigt second-order tensors,

$$\lambda = \frac{1}{15}(2\operatorname{tr}\mathbf{d} - \operatorname{tr}\mathbf{v}) \quad \textit{and} \quad \mu = \frac{1}{30}(3\operatorname{tr}\mathbf{v} - \operatorname{tr}\mathbf{d}),$$

the Lamé constants,

$$\mathbf{H} = \mathbf{E}^s - (2\mu + \lambda)\mathbf{1}\odot\mathbf{1} - \frac{2}{7}\mathbf{1}\odot(\mathbf{d}' + 2\mathbf{v}') \tag{17}$$

and

$$\mathbf{d}_2 = \mathbf{H} \,\vdots\, \mathbf{H},$$

with components $(\mathbf{d}_2)_{ij} = H_{ipqr}H_{pqrj}$*. Then,* $\mathbf{E}$ *is cubic if and only if*

$$\mathbf{d}' = \mathbf{v}' = 0, \qquad \mathbf{d}_2' = 0, \quad \textit{and} \quad J_2 = \operatorname{tr}\mathbf{d}_2 \neq 0.$$

Remark 3.4. The decomposition of any elasticity tensor provided by the above formulas,

$$\mathbf{E} = (\lambda, \mu, \mathbf{d}', \mathbf{v}', \mathbf{H}),$$

into the harmonic components $\lambda, \mu \in \mathbb{H}^0$, $\mathbf{d}', \mathbf{v}' \in \mathbb{H}^2$ and $\mathbf{H} \in \mathbb{H}^4$, is the so-called harmonic decomposition of $\mathbf{E}$ [10, 58, 18].

4. Cubic pair of elasticity-like tensors

There exist constitutive laws (for instance, anisotropic elasto-plasticity [35]) involving two fourth-order constitutive tensors. The question of the characterization of all the symmetry classes of a pair

$$(\mathbf{E}, \mathbf{F}) \in \mathbb{E}\mathrm{la} \times \mathbb{E}\mathrm{la}$$

of elasticity-like tensors seems to be an open one. Nevertheless, this question has a relatively simple answer in the cubic symmetry case, thanks to the harmonic decompositions of both tensors $\mathbf{E}$ and $\mathbf{F}$,

$$\mathbf{E} = (\lambda, \mu, \mathbf{d}', \mathbf{v}', \mathbf{H}) \quad \text{and} \quad \mathbf{F} = (\ell, m, \mathbf{e}', \mathbf{w}', \mathbf{K}),$$

and by recalling that the symmetry group $G_{(\mathbf{E},\mathbf{F})}$ of the pair $(\mathbf{E}, \mathbf{F})$ is the intersection of the symmetry groups of its harmonic components [26],

$$G_{(\mathbf{E},\mathbf{F})} = G_{\mathbf{E}} \cap G_{\mathbf{F}} = G_{\mathbf{d}'} \cap G_{\mathbf{v}'} \cap G_{\mathbf{H}} \cap G_{\mathbf{e}'} \cap G_{\mathbf{w}'} \cap G_{\mathbf{K}}.$$

As an harmonic (deviatoric) cubic second-order tensor is isotropic and therefore vanishes (so that $G_{(\mathbf{E},\mathbf{F})} = G_{\mathbf{H}} \cap G_{\mathbf{K}}$), and as the normal form of an harmonic cubic fourth-order tensor is one-dimensional, the pair of elasticity-like fourth order tensors $(\mathbf{E}, \mathbf{F})$ is cubic if and only if its harmonic second-order components vanish and its harmonic fourth-order components are cubic and proportional. By theorem 3.3 we get the following result.

Theorem 4.1. *Let* $\mathbf{E} = (\lambda, \mu, \mathbf{d}', \mathbf{v}', \mathbf{H}) \in \mathbb{E}\mathrm{la}$ *and* $\mathbf{F} = (\ell, m, \mathbf{e}', \mathbf{w}', \mathbf{K}) \in \mathbb{E}\mathrm{la}$ *be two elasticity-like fourth-order tensors, and*

$$\mathbf{d}_2(\mathbf{H}) = \mathbf{H} \vdots \mathbf{H}, \qquad \mathbf{d}_2(\mathbf{K}) = \mathbf{K} \vdots \mathbf{K},$$

be the quadratic covariants of their respective harmonic fourth-order components $\mathbf{H}$ *and* $\mathbf{K}$*. Then, the pair* $(\mathbf{E}, \mathbf{F})$ *is cubic if and only if*

$$\mathbf{d}' = \mathbf{v}' = \mathbf{e}' = \mathbf{w}' = 0,$$

and either

$$(a) \qquad \mathbf{d}_2'(\mathbf{H}) = 0 \quad \textit{and} \quad \mathbf{H} = k\mathbf{K} \neq 0,$$

or

$$(b) \qquad \mathbf{d}_2'(\mathbf{K}) = 0 \quad \textit{and} \quad \mathbf{K} = k\mathbf{H} \neq 0,$$

with $k \in \mathbb{R}$*.*

5. Distance to cubic elasticity as a quadratic optimization problem

It is possible to reformulate the distance to cubic symmetry problem into a *quadratic optimization problem*

$$\min_{\mathbf{E}} \|\mathbf{E}_0 - \mathbf{E}\|^2 \quad \text{with } \mathbf{E} \text{ at least cubic},$$

since the function to be minimized $\|\mathbf{E}_0 - \mathbf{E}\|^2$ and the constraint "$\mathbf{E}$ at least cubic" (equivalent to $\mathbf{d}' = \mathbf{v}' = 0$ and $\mathbf{d}_2' = 0$ by theorem 3.3) are expressed by quadratic polynomials in $\mathbf{E}$. This 21-dimensional problem can be further reduced to a 9-dimensional optimization problem in the harmonic component $\mathbf{H} \in \mathbb{H}^4$ of $\mathbf{E}$ only.

To achieve this reduction, we perform the harmonic decompositions of both the given and the sought tensors $\mathbf{E}_0$ and $\mathbf{E}$ (see remark 3.4 and (9)),

$$\mathbf{E}_0 = (\lambda_0, \mu_0, \mathbf{d}_0', \mathbf{v}_0', \mathbf{H}_0) \quad \text{and} \quad \mathbf{E} = (\lambda, \mu, 0, 0, \mathbf{H}).$$

Then, using the formula

$$\|\mathbf{E}\|^2 = 3\left(3\lambda^2 + 4\lambda\mu + 8\mu^2\right) + \frac{2}{21}\|\mathbf{d}' + 2\mathbf{v}'\|^2 + \frac{4}{3}\|\mathbf{d}' - \mathbf{v}'\|^2 + \|\mathbf{H}\|^2, \tag{18}$$

for the Euclidean squared norm $\|\mathbf{E}\|^2 := \mathbf{E} :: \mathbf{E}$ of an elasticity tensor $\mathbf{E} = (\lambda, \mu, \mathbf{d}', \mathbf{v}', \mathbf{H})$, we get

$$f(\mathbf{E}) = \|\mathbf{E}_0 - \mathbf{E}\|^2 = 3\left(3(\lambda_0 - \lambda)^2 + 4(\lambda_0 - \lambda)(\mu_0 - \mu) + 8(\mu_0 - \mu)^2\right) + \frac{2}{21}\|\mathbf{d}_0' + 2\mathbf{v}_0'\|^2 + \frac{4}{3}\|\mathbf{d}_0' - \mathbf{v}_0'\|^2 + \|\mathbf{H}_0 - \mathbf{H}\|^2,$$

whose minimum for $\mathbf{E} = \mathbf{E}^*$ cubic is obtained for $\lambda = \lambda_0$, $\mu = \mu_0$ and $\mathbf{H}$ cubic. We have therefore

$$\mathbf{E}^* = 2\mu_0\,\mathbf{I} + \lambda_0 \mathbf{1} \otimes \mathbf{1} + \mathbf{H}^*,$$

with $\mathbf{H}^* \in \mathbb{H}^4$ solution of the quadratic optimization problem

$$\min_{\mathbf{H}} \|\mathbf{H}_0 - \mathbf{H}\|^2 \quad \text{with} \quad g = \mathbf{d}_2' = 0, \tag{19}$$

and the five scalar constraints in (5)

$$(\mathbf{d}_2')_{11} = 0, \quad (\mathbf{d}_2')_{22} = 0, \quad (\mathbf{d}_2')_{12} = 0, \quad (\mathbf{d}_2')_{13} = 0, \quad \text{and} \quad (\mathbf{d}_2')_{23} = 0,$$

are indeed quadratic in $\mathbf{H}$.

The optimum is cubic if $\mathbf{H}^* \neq 0$, with then the *distance* and the *relative distance* to cubic symmetry respectively equal to

$$d(\mathbf{E}_0, \text{cubic symmetry}) = \|\mathbf{E}_0 - \mathbf{E}^*\| = \sqrt{\frac{2}{21}\|\mathbf{d}_0' + 2\mathbf{v}_0'\|^2 + \frac{4}{3}\|\mathbf{d}_0' - \mathbf{v}_0'\|^2 + \|\mathbf{H}_0 - \mathbf{H}^*\|^2},$$

and

$$\frac{d(\mathbf{E}_0, \text{cubic symmetry})}{\|\mathbf{E}_0\|} = \frac{\|\mathbf{E}_0 - \mathbf{E}^*\|}{\|\mathbf{E}_0\|}.$$

In order to apply the Euler–Lagrange method to our constrained optimization problem (19), we have to check (see section 2) that the smooth mapping

$$g : \mathbb{H}^4 \to \mathbb{H}^2, \qquad \mathbf{H} \mapsto \mathbf{d}_2' = (\mathbf{H} \,\vdots\, \mathbf{H})',$$

is a submersion for all cubic tensors $\mathbf{H} \in \mathbb{H}^4$ (*i.e.*, that the Jacobian matrix $T_{\mathbf{H}}g : \mathbb{H}^4 \to \mathbb{H}^2$ is of maximum rank 5, for each cubic tensor $\mathbf{H}$). This is indeed the case. To show this, we observe that the mapping $\mathbf{H} \mapsto g(\mathbf{H}) = (\mathbf{H} \,\vdots\, \mathbf{H})'$ is covariant, meaning that

$$g(Q \star \mathbf{H}) = Q \star g(\mathbf{H})$$

for every rotation Q. Therefore, the rank of $T_{\mathbf{H}}g$ is equal to the rank of $T_{Q\star\mathbf{H}}g$ for every rotation Q and it is enough to compute this rank when $\mathbf{H}$ is the cubic normal form (11), which is 5. Note however that g is not a submersion when $\mathbf{H} = 0$ (*i.e.*, when $\mathbf{H}$ is isotropic).

The Euler–Lagrange method further reduces the distance problem (at given $\mathbf{H}_0$),

$$\min_{g(\mathbf{H})=0} f(\mathbf{H}), \qquad f(\mathbf{H}) = \|\mathbf{H}_0 - \mathbf{H}\|^2, \qquad g(\mathbf{H}) = \mathbf{d}_2',$$

to the determination of the critical points of the polynomial function

$$F(\mathbf{H}, \boldsymbol{\lambda}) = \|\mathbf{H}_0 - \mathbf{H}\|^2 + \boldsymbol{\lambda} : g(\mathbf{H}),$$

with $\mathbf{H} \in \mathbb{H}^4$ an harmonic fourth-order tensor and where the Lagrange multiplier $\boldsymbol{\lambda} \in \mathbb{H}^2$ is an harmonic (deviatoric) second-order tensor.

The differential of F with respect to $\mathbf{H}$ is given by

$$\begin{aligned} \mathrm{d}F.\delta\mathbf{H} &= 2(\mathbf{H} - \mathbf{H}_0) :: \delta\mathbf{H} + \boldsymbol{\lambda} : (\mathbf{H} \,\vdots\, \delta\mathbf{H} + \delta\mathbf{H} \,\vdots\, \mathbf{H}) \\ &= 2(\mathbf{H} - \mathbf{H}_0) :: \delta\mathbf{H} + 2\,\mathbf{S}(\boldsymbol{\lambda}) :: \delta\mathbf{H}, \end{aligned}$$

thanks to the equalities $\boldsymbol{\lambda} : \mathbf{d}_2' = \boldsymbol{\lambda} : \mathbf{d}_2 = \boldsymbol{\lambda} : (\mathbf{H} \,\vdots\, \mathbf{H})$, where

$$\mathbf{S}(\boldsymbol{\lambda}) := \frac{1}{2}\,\mathrm{grad}_{\mathbf{H}}(\boldsymbol{\lambda} : \mathbf{d}_2') = (\mathbf{H} \cdot \boldsymbol{\lambda})^{s\prime} \in \mathbb{H}^4, \tag{20}$$

is the fourth-order harmonic part of the tensor $(\mathbf{H}\cdot\boldsymbol{\lambda})^s$ (of components $H_{ijkp}\lambda_{pl}$). It can be computed using for example Eq. (17), or using directly the harmonic decomposition of totally symmetric tensors [58][52, Section 2.2], with here

$$\operatorname{tr}(\mathbf{H}\cdot\boldsymbol{\lambda})^s = \frac{1}{2}\,\mathbf{H}:\boldsymbol{\lambda} \quad \text{and} \quad \operatorname{tr}\operatorname{tr}(\mathbf{S}(\boldsymbol{\lambda})) = \operatorname{tr}\operatorname{tr}(\mathbf{H}\cdot\boldsymbol{\lambda})^s = 0, \tag{21}$$

so that (introducing the symmetrized tensor product $\odot$)

$$\mathbf{S}(\boldsymbol{\lambda}) = (\mathbf{H}\cdot\boldsymbol{\lambda})^s - \frac{3}{7}\mathbf{1}\odot(\mathbf{H}:\boldsymbol{\lambda}). \tag{22}$$

Therefore, the Euler–Lagrange equations $\dfrac{\partial F}{\partial \mathbf{H}} = 0$ and $\dfrac{\partial F}{\partial \boldsymbol{\lambda}} = 0$ reduce to the system of equations

$$\begin{cases} \mathbf{H} - \mathbf{H}_0 + \mathbf{S}(\boldsymbol{\lambda}) = 0 & \textit{(9 scalar equations)}, \\ \mathbf{d}_2' = 0 & \textit{(5 scalar equations)}, \end{cases} \tag{23}$$

in the 9 independent components H_{ijkl} of $\mathbf{H}\in\mathbb{H}^4$ and the 5 independent components λ_{ij} of $\boldsymbol{\lambda}\in\mathbb{H}^2$.

The system (23) can be further simplified by extracting from the equality $\mathbf{H}-\mathbf{H}_0+\mathbf{S}(\boldsymbol{\lambda})=0$ some linear equations in $\mathbf{H}$.

Lemma 5.1. *The Euler–Lagrange system (23) implies that*

$$\begin{cases} \mathbf{H}\,\vdots\,\mathbf{H}_0 - \mathbf{H}_0\,\vdots\,\mathbf{H} = 0, & \textit{(3 linear scalar equations)} \\ (\mathbf{H}-\mathbf{H}_0)::\mathbf{H} = 0, & \textit{(1 quadratic scalar equation)} \\ \mathbf{d}_2' = 0. & \textit{(5 quadratic scalar equations)} \end{cases} \tag{24}$$

Proof. By contracting three times the first equation $\mathbf{H}-\mathbf{H}_0+\mathbf{S}(\boldsymbol{\lambda})=0$ in (23) with $\mathbf{H}$ on the right and then on the left, we get

$$\mathbf{H}\,\vdots\,\mathbf{H} - \mathbf{H}_0\,\vdots\,\mathbf{H} + \mathbf{S}(\boldsymbol{\lambda})\,\vdots\,\mathbf{H} = 0, \tag{25a}$$

$$\mathbf{H}\,\vdots\,\mathbf{H} - \mathbf{H}\,\vdots\,\mathbf{H}_0 + \mathbf{H}\,\vdots\,\mathbf{S}(\boldsymbol{\lambda}) = 0. \tag{25b}$$

By (22) and some calculations, we have

$$\mathbf{S}(\boldsymbol{\lambda})\,\vdots\,\mathbf{H} = (\mathbf{H}\cdot\boldsymbol{\lambda})^s\,\vdots\,\mathbf{H} - \frac{3}{7}\left(\mathbf{1}\odot(\mathbf{H}:\boldsymbol{\lambda})\right)\vdots\,\mathbf{H} = \frac{1}{4}\boldsymbol{\lambda}\cdot\mathbf{d}_2 + \frac{3}{4}\mathbf{c} - \frac{3}{14}\mathbf{H}^2:\boldsymbol{\lambda}$$

and

$$\mathbf{H}\,\vdots\,\mathbf{S}(\boldsymbol{\lambda}) = \mathbf{H}\,\vdots(\mathbf{H}\cdot\boldsymbol{\lambda})^s - \frac{3}{7}\mathbf{H}\,\vdots\,(\mathbf{1}\odot(\mathbf{H}:\boldsymbol{\lambda})) = \frac{1}{4}\mathbf{d}_2\cdot\boldsymbol{\lambda} + \frac{3}{4}\mathbf{c} - \frac{3}{14}\mathbf{H}^2:\boldsymbol{\lambda}$$

where both $\mathbf{c}$ and $\mathbf{H}^2:\boldsymbol{\lambda} = \mathbf{H}:\mathbf{H}:\boldsymbol{\lambda}$ are symmetric second-order tensors with components

$$c_{ij} = H_{ipqr}H_{jpqs}\lambda_{rs}, \qquad (\mathbf{H}^2:\boldsymbol{\lambda})_{ij} = H_{ijkl}H_{klmn}\lambda_{mn}.$$

If $\mathbf{H}$ is at least cubic, then, $\mathbf{d}_2'=0$ and $\boldsymbol{\lambda}\cdot\mathbf{d}_2 = \mathbf{d}_2\cdot\boldsymbol{\lambda}$ is symmetric. Thus

$$\mathbf{S}(\boldsymbol{\lambda})\,\vdots\,\mathbf{H} = \mathbf{H}\,\vdots\,\mathbf{S}(\boldsymbol{\lambda}),$$

and, substracting (25b) from (25a), we get

$$\mathbf{H}\,\vdots\,\mathbf{H}_0 - \mathbf{H}_0\,\vdots\,\mathbf{H} = 0.$$

The second equation in (24) is obtained, by applying the Euler lemma on homogeneous functions to the quadratic function

$$\mathbf{H}\mapsto\frac{1}{2}\boldsymbol{\lambda}:\mathbf{d}_2'(\mathbf{H}),$$

whose gradient is $\mathbf{S}(\boldsymbol{\lambda})$. We get

$$\mathbf{S}(\boldsymbol{\lambda})::\mathbf{H} = \frac{1}{2}\left(\operatorname{grad}_{\mathbf{H}}(\boldsymbol{\lambda}:\mathbf{d}_2')\right)::\mathbf{H} = \boldsymbol{\lambda}:\mathbf{d}_2'(\mathbf{H}) = 0,$$

for each tensor $\mathbf{H}$ which satisfies $\mathbf{d}_2'(\mathbf{H}) = 0$. Therefore, contracting four times the first equation $\mathbf{H}-\mathbf{H}_0+\mathbf{S}(\boldsymbol{\lambda}) = 0$ in (23) with $\mathbf{H}$, we obtain the second equation of (24), $(\mathbf{H}-\mathbf{H}_0) :: \mathbf{H} = 0$. □

6. Numerical application – Distance to cubic elasticity

Let us now apply the Euler–Lagrange method to the problem of determining the distance

$$d(\mathbf{E}_0, \text{cubic symmetry}) = \min_{\mathbf{E}\,\text{cubic}} \|\mathbf{E}_0 - \mathbf{E}\| = \|\mathbf{E}_0 - \mathbf{E}^*\|,$$

of an experimental tensor $\mathbf{E}_0$ to the cubic symmetry closed stratum. In our application the tensor $\mathbf{E}_0$, taken from [29] (refer to [41, 8, 7, 28, 21, 16] for measurements), is the elasticity tensor of a Nickel-based single crystal superalloy. In Voigt notation:

$$[\mathbf{E}_0] = \begin{pmatrix} 243 & 136 & 135 & 22 & 52 & -17 \\ 136 & 239 & 137 & -28 & 11 & 16 \\ 135 & 137 & 233 & 29 & -49 & 3 \\ 22 & -28 & 29 & 133 & -10 & -4 \\ 52 & 11 & -49 & -10 & 119 & -2 \\ -17 & 16 & 3 & -4 & -2 & 130 \end{pmatrix} \text{ GPa}, \qquad \|\mathbf{E}_0\| = 713.41 \text{ GPa}. \tag{26}$$

It can be checked (by [53, Theorem 10.2], see also [29]) that the tensor $\mathbf{E}_0$ is triclinic (with no material symmetry), even if it corresponds to a material with a so-called cubic γ/γ' microstructure [30, 54, 56].

Using the formulas of theorem 3.3 we obtain the harmonic components of $\mathbf{E}_0$,

$$\lambda_0 = \frac{1583}{15} \text{ GPa}, \qquad \mu_0 = \frac{1453}{15} \text{ GPa},$$

$$\mathbf{d}_0' = \begin{pmatrix} \frac{11}{3} & 2 & 14 \\ 2 & \frac{5}{3} & 23 \\ 14 & 23 & -\frac{16}{3} \end{pmatrix} \text{ GPa}, \qquad \mathbf{v}_0' = \begin{pmatrix} -1 & -11 & -1 \\ -11 & 9 & -1 \\ -1 & -1 & -8 \end{pmatrix} \text{ GPa},$$

and, by (17) (in Voigt notation),

$$[\mathbf{H}_0] = \frac{1}{35} \begin{pmatrix} -1986 & 1093 & 893 & 175 & 1760 & -495 \\ 1093 & -2306 & 1213 & -1085 & 15 & 660 \\ 893 & 1213 & -2106 & 910 & -1775 & -165 \\ 175 & -1085 & 910 & 1213 & -165 & 15 \\ 1760 & 15 & -1775 & -165 & 893 & 175 \\ -495 & 660 & -165 & 15 & 175 & 1093 \end{pmatrix} \text{ GPa}. \tag{27}$$

The cost function $f = \|\mathbf{H}_0 - \mathbf{H}\|^2$ to minimize can then be expressed as (in GPa^2)

$$\begin{aligned} f(\boldsymbol{x}) =& 8\Lambda_1^2 + 2\Lambda_1\Lambda_2 + 2\Lambda_1\Lambda_3 + 668\Lambda_1 + 8\Lambda_2^2 + 2\Lambda_2\Lambda_3 + 540\Lambda_2 + 8\Lambda_3^2 + 620\Lambda_3 \\ &+ 16X_1^2 + 8X_1(X_2 - 11) + 8X_2^2 - 456X_2 + 16Y_1^2 + 8Y_1Y_2 - 392Y_1 \\ &+ 8Y_2^2 - 808Y_2 + 16Z_1^2 + 8Z_1Z_2 - 264Z_1 + 8Z_2^2 - 264Z_2 + \frac{2026042}{35} \end{aligned}$$

in the variable

$$\boldsymbol{x} = (X_1, X_2, Y_1, Y_2, Z_1, Z_2, \Lambda_1, \Lambda_2, \Lambda_3).$$

if the parameterization (10) is used for $\mathbf{H}$.

In terms of components, and according to the expression (26) for the considered material, the system of equations of lemma 5.1 is constituted

(a) *of the three scalar equations,*

$$\begin{aligned} X_1 =& \frac{1515991\Lambda_1 + 6907074\Lambda_2 + 2816520\Lambda_3 + 4774213Y_2 + 1319317Z_1 + 3827136Z_2}{2851559}, \\ X_2 =& \frac{-2752251\Lambda_1 - 5474665\Lambda_2 - 1823999\Lambda_3 - 3665127Y_2 + 1198746Z_1 - 1655027Z_2}{2851559}, \\ Y_1 =& \frac{-1401385\Lambda_1 - 23691851\Lambda_2 - 1939864\Lambda_3 - 15828579Y_2 + 4529623Z_1 + 4531405Z_2}{8554677}, \end{aligned}$$

which correspond to the linear equation $\mathbf{H} \vdots \mathbf{H}_0 - \mathbf{H}_0 \vdots \mathbf{H} = 0$,

(b) *of the scalar equation,*

$$(\mathbf{H}-\mathbf{H}_0) :: \mathbf{H} = 8\Lambda_1^2+2\Lambda_1\Lambda_2+2\Lambda_1\Lambda_3+8\Lambda_2^2+2\Lambda_2\Lambda_3+8\Lambda_3^2+16X_1^2+8X_1X_2+8X_2^2+16Y_1^2+8Y_1Y_2$$
$$+8Y_2^2+16Z_1^2+8Z_1Z_2+8Z_2^2+334\Lambda_1+270\Lambda_2+310\Lambda_3-44X_1-228X_2-196Y_1-404Y_2-132Z_1-132Z_2$$

(c) *and of the 5 equations* $g_{ij} = (\mathbf{d}_2)'_{ij} = 0$, with

$$\begin{aligned}
g_{11} = (\mathbf{d}_2')_{11} =& \frac{2}{3}\big(-4\Lambda_1^2 - \Lambda_1\Lambda_2 - \Lambda_1\Lambda_3 + 2\Lambda_2^2 + 2\Lambda_2\Lambda_3 + 2\Lambda_3^2 + X_1^2 - 4X_1X_2 - 4X_2^2 \\
&+ Y_1^2 + 5Y_1Y_2 + 2Y_2^2 - 2Z_1^2 - Z_1Z_2 + 2Z_2^2\big), \\
g_{22} = (\mathbf{d}_2')_{22} =& -\frac{2}{3}\big(-2\Lambda_1^2 + \Lambda_1\Lambda_2 - 2\Lambda_1\Lambda_3 + 4\Lambda_2^2 + \Lambda_2\Lambda_3 - 2\Lambda_3^2 + 2X_1^2 + X_1X_2 - 2X_2^2 \\
&- Y_1^2 + 4Y_1Y_2 + 4Y_2^2 - Z_1^2 - 5Z_1Z_2 - 2Z_2^2\big), \\
g_{12} = (\mathbf{d}_2')_{12} =& 3X_1Y_1 + 3X_2Y_1 - 4X_1Y_2 - X_2Y_2 + 4Z_1\Lambda_1 + Z_2\Lambda_1 + 3Z_1\Lambda_2 - Z_2\Lambda_2 - 2Z_1\Lambda_3, \\
g_{13} = (\mathbf{d}_2')_{13} =& 3X_1(Z_1 + Z_2) - X_2(4Z_1 + Z_2) + 3Y_1\Lambda_1 - Y_2\Lambda_1 - 2Y_1\Lambda_2 + 4Y_1\Lambda_3 + Y_2\Lambda_3, \\
g_{23} = (\mathbf{d}_2')_{23} =& 3Y_1Z_1 + 3Y_2Z_1 - 4Y_1Z_2 - Y_2Z_2 - 2X_1\Lambda_1 + 4X_1\Lambda_2 + X_2\Lambda_2 + 3X_1\Lambda_3 - X_2\Lambda_3.
\end{aligned}$$

Using the first three linear equations (of point (a)), we further reduce the system to 6 equations

$$g_{ij} = 0 \quad \text{and} \quad g_6 = (\mathbf{H} - \mathbf{H}_0) :: \mathbf{H} = 0,$$

quadratic in the 6 variables $Y_2, Z_1, Z_2, \Lambda_1, \Lambda_2, \Lambda_3$, and which can be solved thanks to the determination of a Gröbner basis GB, by symbolic computation using Mathematica software[3]. We take advantage of the fact that the material parameters (here the components of $\mathbf{E}_0$), are measured with only a few significant digits to work with rational coefficients polynomials. This point is of main importance in the resolution of a system of polynomial equations by the obtention of a Gröbner basis (see remark A.1 of the Appendix). The result is a set $\mathrm{GB} = \{\mathrm{GB}_1, \dots, \mathrm{GB}_{32}\}$ of 32 polynomials GB_n (unfortunately too lengthy to be given) in the variables $Y_2, Z_1, Z_2, \Lambda_1, \Lambda_2, \Lambda_3$, and which vanishes if and only if the initial (polynomial) system (24) is satisfied.

In the present application, the first polynomial of the Gröbner basis GB_1 is found to be function of Λ_3 only, GB_2 function of Λ_2 and Λ_3 (but linear in Λ_2), and so on, up to GB_{32} function of all the variables (but linear in Y_2), as in (38) of Appendix A with $n = 6$ and $x_6 = \Lambda_3$. Solving[4] $\mathrm{GB}_1(\Lambda_3) = 0$, we get either $\Lambda_3 = \Lambda_3^{(0)} = 0$ (leading to the isotropic solution $\mathbf{H}^{(0)} = 0$) or Λ_3 is a real root of a polynomial of degree 14, which has 8 non-zero real roots (in practice determined with a 50 significant digits precision),

$$\begin{aligned}
&\Lambda_3^{(1)} = -38.908854, \quad \Lambda_3^{(2)} = -10.425971, \quad \Lambda_3^{(3)} = -8.424314, \quad \Lambda_3^{(4)} = -6.225368, \\
&\Lambda_3^{(5)} = -3.194952, \quad \Lambda_3^{(6)} = -3.056232, \quad \Lambda_3^{(7)} = 1.745698, \quad \Lambda_3^{(8)} = 13.541284.
\end{aligned}$$

Except from this initial (roots) solving, the remaining unknowns Λ_2, then Λ_1, Z_2, Z_1 and last Y_2, are obtained analytically one per one for each $\Lambda_3^{(s)}$ solution (thanks to the equations $\mathrm{GB}_m = 0$, $m \geq 2$, given by the elements of the Gröbner basis GB, when Λ_3 is evaluated). The variables X_1, X_2, Y_1 are finally given by the three linear equations of point (a).

This polynomial optimization approach shows that, generically, for the distance to cubic symmetry problem, the number of critical points solutions of the first-order Euler–Lagrange equations (24) is finite, the corresponding solutions $\mathbf{H}^{(s)}$ being fully determined by all the roots of the polynomials in the Gröbner basis GB. The global minimum $\min f(\mathbf{H})$ is simply the minimum minimorum

$$\min_{1\leq s\leq 8} \|\mathbf{H}_0 - \mathbf{H}^{(s)}\|^2 = \|\mathbf{H}_0 - \mathbf{H}^{(1)}\|^2 = 2530.47\,\mathrm{GPa}^2,$$

[3]by the command GB = **GroebnerBasis** $[\{g11, g22, g12, g13, g23, g6\}, \{Y2, Z1, Z2, \Lambda1, \Lambda2, \Lambda3\}]$, where by default the lexicographic elimination order is used.

[4]using the command **NSolve**$[\mathrm{GB}[[1]] == 0, \Lambda3, \textbf{WorkingPrecision} \to 50]$.

which is here given by the solution $s = 1$, $\Lambda_3 = \Lambda_3^{(1)}$,

$$X_1 = -6.396655, \qquad X_2 = 27.780761, \qquad Y_1 = -2.277535,$$
$$Y_2 = 44.251233, \qquad Z_1 = -4.557361, \qquad Z_2 = 21.161420,$$
$$\Lambda_1 = -36.401302, \qquad \Lambda_2 = -20.226895, \qquad \Lambda_3 = -38.908854,$$

for $\mathbf{H}^*$. The numerical value $f(0) = \|\mathbf{H}_0\|^2 = 57886.9\,\mathrm{GPa}^2$ for $\mathbf{H}$ isotropic is found larger than the one $2530.47\,\mathrm{GPa}^2$ for the optimal cubic tensor $\mathbf{H}$.

With the values $\lambda = \lambda_0 = 1583/15 = 105.533333$ and $\mu = \mu_0 = 1453/15 = 96.866667$, the tensor

$$\mathbf{E}^* = 2\mu_0\mathbf{I} + \lambda_0\mathbf{1}\otimes\mathbf{1} + \mathbf{H}^*,$$

of Voigt representation

$$[\mathbf{E}^*] = \begin{pmatrix} 240.130916 & 144.442188 & 125.760229 & 6.39665526 & 41.9736976 & -21.1614201 \\ 144.442188 & 223.956510 & 141.934636 & -27.7807617 & 2.27753546 & 16.6040582 \\ 125.760229 & 141.934636 & 242.638469 & 21.3841064 & -44.2512331 & 4.55736193 \\ 6.39665526 & -27.7807617 & 21.3841064 & 133.267969 & 4.55736193 & 2.27753546 \\ 41.9736976 & 2.27753546 & -44.2512331 & 4.55736193 & 117.093562 & 6.39665526 \\ -21.1614201 & 16.6040582 & 4.55736193 & 2.27753546 & 6.39665526 & 135.775521 \end{pmatrix} \mathrm{GPa} \tag{28}$$

is the (cubic) elasticity tensor that minimizes the distance to cubic symmetry, with then

$$d(\mathbf{E}_0, \text{cubic symmetry}) = 74.13 \ \ \mathrm{GPa}.$$

With a relative distance

$$\frac{\|\mathbf{E}_0 - \mathbf{E}^*\|}{\|\mathbf{E}_0\|} = 0.1039,$$

it is slightly better than the solution obtained by François–Geymonat–Berthaud by a numerical iterative method [29].

As $\mathbf{H}^* \neq 0$, the tensor $\mathbf{E}^*$ is cubic. The distance of $\mathbf{E}_0$ to isotropy,

$$d(\mathbf{E}_0, \text{isotropy}) = \|\mathbf{E}_0 - (2\mu_0\mathbf{I} + \lambda_0\mathbf{1}\otimes\mathbf{1})\| = 246.68 \ \ \mathrm{GPa},$$

is found larger than the one to cubic symmetry, with a relative distance to isotropy

$$\frac{d(\mathbf{E}_0, \text{isotropy})}{\|\mathbf{E}_0\|} = 0.3458.$$

By remark 3.2, the normal form (denoted here by $\mathbf{E}^*_{\mathbb{O}}$) of the optimal cubic elasticity tensor $\mathbf{E}^* = (\lambda = \lambda_0, \mu = \mu_0, 0, 0, \mathbf{H}^*)$ given by (28), is obtained directly thanks to the computation of its invariants. We get, by the explicit formulas (12) to (15),

$$J_2 = \|\mathbf{H}^*\|^2 = 55356.440\,\mathrm{GPa}^2, \qquad J_3 = \mathrm{tr}_{13}(\mathbf{H}^{*\,3}) = -2377889.1\,\mathrm{GPa}^3,$$

so that, in GPa,

$$\lambda = 105.533333, \qquad \mu = 96.866667, \qquad \delta = \frac{J_3}{4J_2} = -10.738990,$$

and

$$[\mathbf{E}^*_{\mathbb{O}}] = \begin{pmatrix} 213.354743 & 148.489295 & 148.489295 & 0 & 0 & 0 \\ 148.489295 & 213.354743 & 148.489295 & 0 & 0 & 0 \\ 148.489295 & 148.489295 & 213.354743 & 0 & 0 & 0 \\ 0 & 0 & 0 & 139.822628 & 0 & 0 \\ 0 & 0 & 0 & 0 & 139.822628 & 0 \\ 0 & 0 & 0 & 0 & 0 & 139.822628 \end{pmatrix}_{(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)} \mathrm{GPa}, \tag{29}$$

which, for practical applications, can be by approximated by

$$[\mathbf{E}^*_{\mathbb{O}}] = \begin{pmatrix} 213 & 148.5 & 148.5 & 0 & 0 & 0 \\ 148.5 & 213 & 148.5 & 0 & 0 & 0 \\ 148.5 & 148.5 & 213 & 0 & 0 & 0 \\ 0 & 0 & 0 & 140 & 0 & 0 \\ 0 & 0 & 0 & 0 & 140 & 0 \\ 0 & 0 & 0 & 0 & 0 & 140 \end{pmatrix}_{(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)} \mathrm{GPa}. \tag{30}$$

7. Distance to cubic elasto-plasticity as a polynomial optimization problem

The anisotropic Hill elasto-plasticity theory for metallic materials introduces not one but two fourth-order constitutive tensors [35, 45, 36, 13],

- a first one, $\mathbf{E} \in \mathbb{E}\mathrm{la}$, to describe the anisotropic elasticity,
- a second one, $\mathbf{P}$ (sometimes considered as dimensionless), to describe the yield (plasticity) criterion, and such as the condition

$$\boldsymbol{\sigma}' : \mathbf{P} : \boldsymbol{\sigma}' - R^2 < 0$$

  corresponds to an elastic loading or unloading stage (with $\boldsymbol{\sigma}' \in \mathbb{H}^2$ the continuum mechanics deviatoric stress tensor). When assumed constant, the scalar R stands for the material yield stress, when taken as evolving during loading, it stands for the material hardening. The Hill tensor $\mathbf{P}$ has the indicial symmetries of elasticity tensors (so that $\mathbf{P} \in \mathbb{E}\mathrm{la}$).

With no lack of generality, instead of $\mathbf{P}$, we can work with a tensor $\mathbf{F}$ of elasticity-type, and compute a dimensionless Hill tensor $\mathbf{P} = \mathbf{F}/C$ by normalizing afterward $\mathbf{F}$ with a constant C. Indeed, when $\mathbf{F}$ is in its normal form (8), setting

$$C := \frac{2}{3}(F_{1111} - F_{1122}) \quad \text{and} \quad L := \frac{3F_{1212}}{F_{1111} - F_{1122}}, \tag{31}$$

allows to recover the standard expression of cubic Hill yield criterion (in cubic basis $(\boldsymbol{e}_i)$), as

$$\boldsymbol{\sigma}' : \mathbf{P} : \boldsymbol{\sigma}' = \frac{1}{2}\left((\sigma_{11} - \sigma_{22})^2 + (\sigma_{33} - \sigma_{11})^2 + (\sigma_{22} - \sigma_{33})^2\right) + 2L\left(\sigma_{12}^2 + \sigma_{13}^2 + \sigma_{23}^2\right).$$

The harmonic decomposition of $\mathbf{F}$ is then (see remark 3.4)

$$\mathbf{F} = \left(\ell, m, \mathbf{e}', \mathbf{w}', \mathbf{K}\right),$$

with

$$\ell = \frac{1}{15}(2\,\mathrm{tr}\,\mathbf{e} - \mathrm{tr}\,\mathbf{w}) \quad \text{and} \quad m = \frac{1}{30}(3\,\mathrm{tr}\,\mathbf{w} - \mathrm{tr}\,\mathbf{e}),$$

the Lamé constants of $\mathbf{F}$, where

$$\mathbf{e} := \mathrm{tr}_{12}\,\mathbf{F} \quad \text{and} \quad \mathbf{w} := \mathrm{tr}_{13}\,\mathbf{F},$$

are respectively the dilatation and Voigt tensors of $\mathbf{F}$, and $\mathbf{K} = (\mathbf{F})^{s\prime} \in \mathbb{H}^4$ is the harmonic fourth-order component of $\mathbf{F}$, given by (17),

$$\mathbf{K} = (\mathbf{F})^s - (2m + \ell)\mathbf{1} \odot \mathbf{1} - \frac{2}{7}\mathbf{1} \odot (\mathbf{e}' + 2\mathbf{w}').$$

We now assume that two given elasto-plasticity tensors $\mathbf{E}_0$ and $\mathbf{F}_0$ are available (possibly triclinic) for a given metallic material. As a generalization of the formulation of the distance problem of section 5, in which only one constitutive tensor (the elasticity tensor) was involved, we propose to define the optimum cubic estimates $\mathbf{E}^{**}$ and $\mathbf{F}^{**} = C\mathbf{P}^{**}$ of the two elasto-plasticity constitutive tensors, as the minimizers of the following quadratic function (with W a given strictly positive weight)

$$f(\mathbf{E}, \mathbf{F}) := \|\mathbf{E}_0 - \mathbf{E}\|^2 + W\|\mathbf{F}_0 - \mathbf{F}\|^2,$$

at given tensors $\mathbf{E}_0$ and $\mathbf{F}_0 = C\mathbf{P}_0$, under the constraint that both the elasticity tensor $\mathbf{E}$ and the Hill tensor $\mathbf{F} = C\mathbf{P}$ are cubic and share the same cubic axes (by theorem 4.1). The introduction of a weight W is necessary in practice, since the orders of magnitude (and the units) of the Hooke and Hill tensors are often very different.

Remark 7.1. $\sqrt{\|\mathbf{E}\|^2 + W\|\mathbf{F}\|^2}$, with $W > 0$, is a norm on $\mathbb{E}\mathrm{la} \oplus \mathbb{E}\mathrm{la}$.

We first perform the harmonic decompositions of $\mathbf{E}_0$ and $\mathbf{F}_0$,

$$\mathbf{E}_0 = \left(\lambda_0, \mu_0, \mathbf{d}_0', \mathbf{v}_0', \mathbf{H}_0\right), \qquad \mathbf{F}_0 = \left(\ell_0, m_0, \mathbf{e}_0', \mathbf{w}_0', \mathbf{K}_0\right),$$

with $\lambda_0, \mu_0, \ell_0, m_0 \in \mathbb{H}^0$, $\mathbf{d}_0', \mathbf{v}_0', \mathbf{e}_0', \mathbf{w}_0' \in \mathbb{H}^2$ and $\mathbf{H}_0, \mathbf{K}_0 \in \mathbb{H}^4$ their harmonic components. The harmonic decompositions of the sought cubic tensors $\mathbf{E}$ and $\mathbf{F}$ are

$$\mathbf{E} = (\lambda, \mu, 0, 0, \mathbf{H}), \qquad \mathbf{F} = (\ell, m, 0, 0, \mathbf{K}),$$

with $\lambda, \mu, \ell, m \in \mathbb{H}^0$, $\mathbf{H}, \mathbf{K} \in \mathbb{H}^4$, and, according to (9), we have

$$\mathbf{E} = 2\mu\mathbf{I} + \lambda\mathbf{1} \otimes \mathbf{1} + \mathbf{H} \quad \text{and} \quad \mathbf{F} = 2m\mathbf{I} + \ell\mathbf{1} \otimes \mathbf{1} + \mathbf{K},$$

with $\mathbf{d}_2'(\mathbf{H}) = \mathbf{d}_2'(\mathbf{K}) = 0$ and $\mathbf{K} = k\mathbf{H}$ (by theorem 3.3). Using the formula (18) for both $\|\mathbf{E}_0 - \mathbf{E}\|^2$ and $\|\mathbf{F}_0 - \mathbf{F}\|^2$, we get

$$\begin{aligned} f(\mathbf{E}) = {} & 3\left(3(\lambda_0 - \lambda)^2 + 4(\lambda_0 - \lambda)(\mu_0 - \mu) + 8(\mu_0 - \mu)^2\right) \\ & + 3W\left(3(\ell_0 - \ell)^2 + 4(\ell_0 - \ell)(m_0 - m) + 8(m_0 - m)^2\right) \\ & + \frac{2}{21}\|\mathbf{d}_0' + 2\mathbf{v}_0'\|^2 + \frac{4}{3}\|\mathbf{d}_0' - \mathbf{v}_0'\|^2 + \frac{2W}{21}\|\mathbf{e}_0' + 2\mathbf{w}_0'\|^2 + \frac{4W}{3}\|\mathbf{e}_0' - \mathbf{w}_0'\|^2 \\ & + \|\mathbf{H}_0 - \mathbf{H}\|^2 + W\|\mathbf{K}_0 - k\mathbf{H}\|^2. \end{aligned}$$

The minimum of this expression is obtained for

$$\lambda = \lambda_0, \quad \mu = \mu_0, \quad \ell = \ell_0, \quad m = m_0, \quad \mathbf{H} = \mathbf{H}^*, \quad k = k^*,$$

where $\mathbf{H}^*$ and k^* correspond to absolute minima of the problem

$$\min_{\mathbf{H},k} \left\{\|\mathbf{H}_0 - \mathbf{H}\|^2 + W\|\mathbf{K}_0 - k\mathbf{H}\|^2\right\}, \quad \text{with} \quad \mathbf{d}_2'(\mathbf{H}) = (\mathbf{H} \vdots \mathbf{H})' = 0.$$

Remark 7.2. Note that the condition $\mathbf{K} = k\mathbf{H} \neq 0$ implies that the pair $(\mathbf{H}, \mathbf{K})$ is cubic, meaning that both $\mathbf{H}$ and $\mathbf{K}$ are cubic and share the same cubic axes.

To solve the problem of the distance of a pair $(\mathbf{E}_0, \mathbf{F}_0)$ to cubic symmetry, we therefore have to find the critical points of the polynomial function

$$F(\mathbf{H}, k, \boldsymbol{\lambda}) := \|\mathbf{H}_0 - \mathbf{H}\|^2 + W\|\mathbf{K}_0 - k\mathbf{H}\|^2 + \boldsymbol{\lambda} : g, \tag{32}$$

with $\mathbf{H} \in \mathbb{H}^4$ an harmonic fourth-order tensor, k a scalar, and where the Lagrange multiplier $\boldsymbol{\lambda} \in \mathbb{H}^2$ is a deviatoric second-order tensor. Observe that the first-order Euler–Lagrange equations for this optimization problem can furthermore be recast in a similar form as (24).

Lemma 7.3. *The first-order Euler–Lagrange equations,*

$$\frac{\partial F}{\partial \mathbf{H}} = 0, \quad \frac{\partial F}{\partial k} = 0 \quad \textit{and} \quad \frac{\partial F}{\partial \boldsymbol{\lambda}} = 0,$$

imply

$$\begin{cases} \mathbf{H} \vdots (\mathbf{H}_0 + kW\mathbf{K}_0) - (\mathbf{H}_0 + kW\mathbf{K}_0) \vdots \mathbf{H} = 0 & \textit{(3 scalar equations)} \\ (\mathbf{H} - \mathbf{H}_0) :: \mathbf{H} = 0 & \textit{(1 scalar equation)} \\ W(k\mathbf{H} - \mathbf{K}_0) :: \mathbf{H} = 0 & \textit{(1 scalar equation)} \\ \mathbf{d}_2' = 0 & \textit{(5 scalar equations)} \end{cases} \tag{33}$$

Remark 7.4. The distance problem thus formulated is not a quadratic optimization problem. The equation

$$(k\mathbf{H} - \mathbf{K}_0) :: \mathbf{H} = 0$$

is indeed polynomial, but of degree three in the variable $\boldsymbol{x} = (\mathbf{H}, k)$.

The first equation of (33) is not linear anymore, it cannot be used to reduce the number of unknowns before the computation of a Gröbner basis. The quasi-analytical resolution by the obtention of a Gröbner basis will nevertheless be similar (but with four more variables) to the resolution for the single elasticity tensor case (except that the computation of a Gröbner basis will be more computer time consuming).

8. Numerical application – Distance to cubic elasto-plasticity

We consider here the example of the triclinic elasticity tensor $\mathbf{E}_0$ (still given by (26), the harmonic decomposition $\mathbf{E}_0 = (\lambda_0, \mu_0, \mathbf{d}_0', \mathbf{w}', \mathbf{H}_0)$ remaining the one of section 6), and of the following triclinic plasticity tensor $\mathbf{F}_0$, in Voigt notation,

$$[\mathbf{F}_0] = \begin{pmatrix} 191 & -54 & -83 & -34 & -94 & 59 \\ -54 & 176 & -71 & 71 & -40 & -23 \\ -83 & -71 & 207 & -44 & 130 & -36 \\ -34 & 71 & -44 & 99 & -15 & -17 \\ -94 & -40 & 130 & -15 & 179 & -40 \\ 59 & -23 & -36 & -17 & -40 & 79 \end{pmatrix}, \qquad \|\mathbf{F}_0\| = 715.78.$$

Using the formulas of theorem 3.3, we obtain $\mathbf{F}_0 = (\ell_0, m_0, \mathbf{e}_0', \mathbf{w}_0', \mathbf{K}_0)$, with

$$\ell_0 = -\frac{324}{5}, \qquad m_0 = \frac{1853}{15},$$

$$\mathbf{e}_0' = (\mathrm{tr}_{12}\,\mathbf{F}_0)' = \begin{pmatrix} \frac{4}{3} & 0 & -4 \\ 0 & -\frac{5}{3} & -7 \\ -4 & -7 & \frac{1}{3} \end{pmatrix}, \quad \mathbf{w}_0' = (\mathrm{tr}_{13}\,\mathbf{F}_0)' = \begin{pmatrix} \frac{59}{3} & 21 & 19 \\ 21 & -\frac{226}{3} & -13 \\ 19 & -13 & \frac{167}{3} \end{pmatrix}.$$

and (in Voigt notation)

$$[\mathbf{K}_0] = \frac{1}{35}\begin{pmatrix} -101 & -727 & 828 & -1275 & -3460 & 1855 \\ -727 & 1304 & -577 & 2650 & -920 & -1015 \\ 828 & -577 & -251 & -1375 & 4380 & -840 \\ -1275 & 2650 & -1375 & -577 & -840 & -920 \\ -3460 & -920 & 4380 & -840 & 828 & -1275 \\ 1855 & -1015 & -840 & -920 & -1275 & -727 \end{pmatrix}.$$

The cost function

$$f(\mathbf{H}) = \|\mathbf{H}_0 - \mathbf{H}\|^2 + W\|\mathbf{K}_0 - k\mathbf{H}\|^2,$$

that we have to minimize in order to solve the distance problem

$$\min_{(\mathbf{E},\mathbf{F})\,\mathrm{cubic}} \left(\|\mathbf{E}_0 - \mathbf{E}\|^2 + W\|\mathbf{F}_0 - \mathbf{F}\|^2\right),$$

is (in GPa^2)

$$\begin{aligned} f(\boldsymbol{x}) = {} & 8\Lambda_1^2 + 2\Lambda_1\Lambda_2 + 2\Lambda_1\Lambda_3 + 668\Lambda_1 + 8\Lambda_2^2 + 2\Lambda_2\Lambda_3 + 540\Lambda_2 + 8\Lambda_3^2 + 620\Lambda_3 \\ & + 16X_1^2 + 8X_1(X_2 - 11) + 8X_2^2 - 456X_2 + 16Y_1^2 + 8Y_1Y_2 - 392Y_1 \\ & + 8Y_2^2 - 808Y_2 + 16Z_1^2 + 8Z_1Z_2 - 264Z_1 + 8Z_2^2 - 264Z_2 + \frac{2026042}{35} \\ & + W\Big(16X_1^2k^2 + 8X_1k(X_2k - 70) + 8X_2^2k^2 + 920X_2k + 16Y_1^2k^2 + 8Y_1Y_2k^2 + 160Y_1k \\ & + 8Y_2^2k^2 + 1792Y_2k + 8\Lambda_1^2k^2 + 2\Lambda_1\Lambda_2k^2 + 2\Lambda_1\Lambda_3k^2 + 8\Lambda_2^2k^2 + 2\Lambda_2\Lambda_3k^2 + 8\Lambda_3^2k^2 + 16k^2Z_1^2 \\ & + 8k^2Z_1Z_2 + 8k^2Z_2^2 - 258\Lambda_1k + 304\Lambda_2k - 318\Lambda_3k - 344kZ_1 + 656kZ_2 + \frac{6495682}{35}\Big). \end{aligned}$$

It is expressed in the variable

$$\boldsymbol{x} = (k, X_1, X_2, Y_1, Y_2, Z_1, Z_2, \Lambda_1, \Lambda_2, \Lambda_3),$$

if the parameterization (10) is used for $\mathbf{H}$. The first-order Euler-Lagrange equations are given in lemma 7.3. In components, they consist of

(a) *the three scalar equations,*

$$
\begin{aligned}
(a1)\quad & -43k\Lambda_1 W + 125k\Lambda_2 W + 328k\Lambda_3 W + X_1(199-264kW) + X_2(52-204kW) \\
& - 555kWY_1 - 70kWY_2 + 220kWZ_1 + 159kWZ_2 - 33\Lambda_1 - 132\Lambda_3 + 138Y_1 \\
& - 11Y_2 - 187Z_1 - 310Z_2 = 0, \\
(a2)\quad & kW(-204\Lambda_1 - 896\Lambda_2 - 20\Lambda_3 + 375X_1 + 43X_2 + 61Y_1 + 152Y_2 - 25Z_1 + 185Z_2) \\
& + 52\Lambda_1 + 404\Lambda_2 + 49\Lambda_3 + 33X_2 + 123Y_1 + 270Y_2 - 79Z_1 - 46Z_2 = 0, \\
(a3)\quad & 460k\Lambda_1 W - 70k\Lambda_2 W + 185k\Lambda_3 W - 7X_1(13kW+21) + X_2(129kW-334) \\
& + 4kWY_1 - 125kWY_2 - 612kWZ_1 + 20kWZ_2 - 228\Lambda_1 - 11\Lambda_2 - 46\Lambda_3 \\
& + 99Y_1 + 156Z_1 - 49Z_2 = 0,
\end{aligned}
$$

which correspond to the linear equation $\mathbf{H} \vdots (\mathbf{H}_0 + kW\mathbf{K}_0) - (\mathbf{H}_0 + kW\mathbf{K}_0) \vdots \mathbf{H} = 0$,

(b) *the scalar equation* $(\mathbf{H} - \mathbf{H}_0) :: \mathbf{H} = 0$ (detailed in point (b) of section 6),

(c) *the scalar equation*

$$
\begin{aligned}
(k\mathbf{H} - \mathbf{K}_0) :: \mathbf{H} = {} & 8k\Lambda_1^2 + 2k\Lambda_1\Lambda_2 + 2k\Lambda_1\Lambda_3 + 8k\Lambda_2^2 + 2k\Lambda_2\Lambda_3 + 8k\Lambda_3^2 + 16kX_1^2 \\
& + 8X_1(kX_2 - 35) + 8kX_2^2 + 16kY_1^2 + 8kY_1Y_2 + 8kY_2^2 + 16kZ_1^2 \\
& + 8kZ_1Z_2 + 8kZ_2^2 - 129\Lambda_1 + 152\Lambda_2 - 159\Lambda_3 + 460X_2 + 80Y_1 \\
& + 896Y_2 - 172Z_1 + 328Z_2 \\
= {} & 0,
\end{aligned}
$$

(d) *and the 5 equations* $g_{ij} = (\mathbf{d}_2)'_{ij} = 0$ (detailed in point (c) of section 6).

We set a unit weight $W = 1$ for the numerical application. The resolution is similar to the one for the single elasticity tensor case, except that now the variable $\boldsymbol{x}$ is 10-dimensional, and that there is no *a priori* reduction in the number of scalar unknowns. Rational coefficients are considered for the given tensors $\mathbf{E}_0$ and $\mathbf{F}_0$ (and for their harmonic components $\mathbf{H}_0$ and $\mathbf{K}_0$). A Gröbner basis $\mathrm{GB} = \{\mathrm{GB}_1, \ldots, \mathrm{GB}_{111}\}$ of 111 elements is computed using Mathematica. Its first element GB_1 is found to be a polynomial in Λ_3 only; Λ_3 is either zero (leading to the isotropic solution $\mathbf{H} = 0$) or it is a solution of a polynomial equation of degree 56, which has 18 real non zero roots (in practice determined with a 100 significant digits precision). Once $\mathrm{GB}_1(\Lambda_3) = 0$ is solved, the remaining Gröbner basis equations are linear (as in (38) of Appendix A) in the variables Λ_2, Λ_1, ..., X_2, X_1, and k.

The minimum minimorum for the cost function is here given by the solution $\Lambda_3 = -19.612165$ (it is not given by the isotropic solution $\mathbf{H} = \mathbf{K} = 0$). We get the optimal value $k^{**} = -2.134021$ for k and (in GPa):

$$
\begin{aligned}
X_1 &= -16.788457, & X_2 &= 39.191663, & Y_1 &= -8.812379, \\
Y_2 &= 43.001809, & Z_1 &= -8.048394, & Z_2 &= 30.315189, \\
\Lambda_1 &= -15.769513, & \Lambda_2 &= 5.950665, & \Lambda_3 &= -19.612165,
\end{aligned}
$$

so that the optimal tensor $\mathbf{H}^{**}$ has expression (in Voigt notation)

$$
[\mathbf{H}^{**}] = \begin{pmatrix}
-13.661500 & 19.612165 & -5.950665 & 16.788457 & 34.189430 & -30.315189 \\
19.612165 & -35.381678 & 15.769513 & -39.191663 & 8.812379 & 22.266795 \\
-5.950665 & 15.769513 & -9.818848 & 22.403206 & -43.001809 & 8.048394 \\
16.788457 & -39.191663 & 22.403206 & 15.769513 & 8.048394 & 8.812379 \\
34.189430 & 8.812379 & -43.001809 & 8.048394 & -5.950665 & 16.788457 \\
-30.315189 & 22.266795 & 8.048394 & 8.812379 & 16.788457 & 19.612165
\end{pmatrix} \text{GPa}.
$$

With the values $\lambda = \lambda_0 = 105.533333$ and $\mu = \mu_0 = 96.866667$, the optimal cubic elasticity tensor

$$
\mathbf{E}^{**} = 2\mu_0\mathbf{I} + \lambda_0\mathbf{1} \otimes \mathbf{1} + \mathbf{H}^{**},
$$

has Voigt representation,

$$[\mathbf{E}^{**}] = \begin{pmatrix} 285.605167 & 125.145498 & 99.582668 & 16.788457 & 34.189430 & -30.315189 \\ 125.145498 & 263.884989 & 121.302846 & -39.191663 & 8.812379 & 22.266795 \\ 99.582668 & 121.302846 & 289.447819 & 22.403206 & -43.001809 & 8.048394 \\ 16.788457 & -39.191663 & 22.403206 & 112.636180 & 8.048394 & 8.812379 \\ 34.189430 & 8.812379 & -43.001809 & 8.048394 & 90.916002 & 16.788457 \\ -30.315189 & 22.266795 & 8.048394 & 8.812379 & 16.788457 & 116.478831 \end{pmatrix} \text{GPa}.$$

Since $\ell = \ell_0 = -64.800000$ and $m = m_0 = 123.533333$, we get for the optimal cubic plasticity tensor

$$\mathbf{F}^{**} = 2m_0\mathbf{I} + \ell_0\mathbf{1} \otimes \mathbf{1} + k^{**}\mathbf{H}^{**},$$

the Voigt representation

$$[\mathbf{F}^{**}] = \begin{pmatrix} 211.420595 & -106.652774 & -52.101155 & -35.826922 & -72.960965 & 64.693254 \\ -106.652774 & 257.771914 & -98.452474 & 83.635836 & -18.805804 & -47.517810 \\ -52.101155 & -98.452474 & 203.220295 & -47.808914 & 91.766769 & -17.175444 \\ -35.826922 & 83.635836 & -47.808914 & 89.880860 & -17.175444 & -18.805804 \\ -72.960965 & -18.805804 & 91.766769 & -17.175444 & 136.232178 & -35.826922 \\ 64.693254 & -47.517810 & -17.175444 & -18.805804 & -35.826922 & 81.680560 \end{pmatrix}.$$

The relative distance to cubic symmetry for this two constitutive elasto-plasticity tensors problem is

$$\sqrt{\frac{\|\mathbf{E}_0 - \mathbf{E}^{**}\|^2 + \|\mathbf{F}_0 - \mathbf{F}^{**}\|^2}{\|\mathbf{E}_0\|^2 + \|\mathbf{F}_0\|^2}} = 0.2462.$$

It is slightly larger than the relative distance for the single elasticity tensor case solved in section 6.

As $\mathbf{H}^{**}$ and $\mathbf{K}^{**} = k^{**}\mathbf{H}^{**}$ are non zero, the two optimal tensors $\mathbf{E}^{**}$ and $\mathbf{F}^{**}$ are cubic (and so is the pair $(\mathbf{E}^{**}, \mathbf{F}^{**})$). The relative distance of the given pair $(\mathbf{E}_0, \mathbf{F}_0)$ to isotropy,

$$\sqrt{\frac{\|\mathbf{E}_0 - (2\mu_0\mathbf{I} + \lambda_0\mathbf{1} \otimes \mathbf{1})\|^2 + \|\mathbf{F}_0 - (2m_0\mathbf{I} + \ell_0\mathbf{1} \otimes \mathbf{1})\|^2}{\|\mathbf{E}_0\|^2 + \|\mathbf{F}_0\|^2}} = 0.5096,$$

is larger than the one to cubic symmetry.

The normal forms (8) for both the optimal Hooke and Hill tensors are finally obtained thanks to the computation of their invariants λ, μ J_2, J_3 and δ, here evaluated first for $\mathbf{E}^{**}$ and then for $\mathbf{F}^{**}$ (by remark 3.2). Using (16) for each tensor $\mathbf{E}^{**}$ and $\mathbf{F}^{**}$, we get:

$$[\mathbf{E}^{**}_{\mathbb{O}}] = \begin{pmatrix} 229.484303 & 140.424515 & 140.424515 & 0 & 0 & 0 \\ 140.424515 & 229.484303 & 140.424515 & 0 & 0 & 0 \\ 140.424515 & 140.424515 & 229.484303 & 0 & 0 & 0 \\ 0 & 0 & 0 & 131.757849 & 0 & 0 \\ 0 & 0 & 0 & 0 & 131.757849 & 0 \\ 0 & 0 & 0 & 0 & 0 & 131.757849 \end{pmatrix}_{(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)} \text{GPa},$$

$$[\mathbf{F}^{**}_{\mathbb{O}}] = \begin{pmatrix} 331.183705 & -139.258519 & -139.258519 & 0 & 0 & 0 \\ -139.258519 & 331.183705 & -139.258519 & 0 & 0 & 0 \\ -139.258519 & -139.258519 & 331.183705 & 0 & 0 & 0 \\ 0 & 0 & 0 & 49.074814 & 0 & 0 \\ 0 & 0 & 0 & 0 & 49.074814 & 0 \\ 0 & 0 & 0 & 0 & 0 & 49.074814 \end{pmatrix}_{(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)} \text{GPa},$$

which can be approximated as

$$[\mathbf{E}^{**}_{\mathbb{O}}] = \begin{pmatrix} 229.5 & 140.5 & 140.5 & 0 & 0 & 0 \\ 140.5 & 229.5 & 140.5 & 0 & 0 & 0 \\ 140.5 & 140.5 & 229.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 132 & 0 & 0 \\ 0 & 0 & 0 & 0 & 132 & 0 \\ 0 & 0 & 0 & 0 & 0 & 132 \end{pmatrix}_{(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)} \quad \text{GPa},$$

$$[\mathbf{F}^{**}_{\mathbb{O}}] = \begin{pmatrix} 331 & -139 & -139 & 0 & 0 & 0 \\ -139 & 331 & -139 & 0 & 0 & 0 \\ -139 & -139 & 331 & 0 & 0 & 0 \\ 0 & 0 & 0 & 49 & 0 & 0 \\ 0 & 0 & 0 & 0 & 49 & 0 \\ 0 & 0 & 0 & 0 & 0 & 49 \end{pmatrix}_{(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)} \quad \text{GPa}.$$

These two normal forms are obtained in the same cubic basis $(\boldsymbol{e}_i)$. Finally, by (31), the Hill parameter associated with $\mathbf{F}^{**}_{\mathbb{O}}$ is

$$L = 0.312949 \approx 0.31.$$

9. Recovering the natural basis of a cubic fourth-order constitutive tensor

A continuum mechanics anisotropic constitutive law, such as elasticity, is not represented by a unique constitutive tensor $\mathbf{E}$ but by the set of all elasticity tensors $Q \star \mathbf{E}$ related to $\mathbf{E}$ by a rotation Q. Mathematically speaking, the anisotropic material property is represented by the orbit

$$\mathrm{Orb}(\mathbf{E}) = \{Q \star \mathbf{E},\ \det Q = 1\}.$$

For a given cubic elasticity tensor $\mathbf{E}$, there exists a tensor $\mathbf{E}_{\mathbb{O}}$ in its orbit that is fixed by all the transformations of the orientation preserving octahedral group $\mathbb{O}$. The tensor $\mathbf{E}_{\mathbb{O}}$ is the so-called *normal form* of $\mathbf{E}$, and has (8) as Voigt representation.

When a cubic constitutive tensor – such as the tensors $\mathbf{E}^*$, $\mathbf{E}^{**}$ and $\mathbf{F}^{**}$ of previous numerical applications sections – is not expressed in its natural (cubic) basis, one needs

(1) to compute its normal form,
(2) and to compute the rotation Q that puts it in its normal form.

Task (1) can be done in a straightforward manner, using *Invariant Theory* (see remark 3.2). Note that the polynomial (λ, μ, J_2 and J_3) and rational (δ) invariants then involved are computed in the working basis (in which are expressed $\mathbf{E}^*$, $\mathbf{E}^{**}$ and $\mathbf{F}^{**}$) by explicit formulas, whereas the methodology proposed in [59] needs the computation of the eigenvalues of the Kelvin 6×6 matrix representation of the considered elasticity tensor.

In practice, there are several ways to perform task (2): using *Maxwell multipoles* [11] and solving a degree-8 polynomial equation in one variable, or solving the linear system [2, Appendix B]

$$\mathbf{L}(\mathbf{a}) := \mathrm{tr}(\mathbf{H} \times \mathbf{a}) = 0, \qquad \mathbf{a} \in \mathbb{H}^2,$$

where $\mathbf{H}$ is the fourth-order harmonic component of the considered (cubic) elasticity tensor $\mathbf{E}$ (it will next be either $\mathbf{H}^*$ or $\mathbf{H}^{**}$ or $\mathbf{K}^{**}$). Here, the product $\times$ is the generalized cross product between totally symmetric tensors, defined by (3), and the totally symmetric fifth-order tensor $\mathbf{H} \times \mathbf{a}$ has components

$$(\mathbf{H} \times \mathbf{a})_{ijklm} = (a_{ir}\varepsilon_{rjs}H_{sklm})^s.$$

Generically, the deviatoric tensor $\mathbf{a}$, solution of the equation $\mathbf{L}(\mathbf{a}) = 0$, is orthotropic and carries the cubic basis $(\boldsymbol{e}_i)$. We shall apply the second methodology, which reduces to solve the linear equation $\mathbf{L}(\mathbf{a}) = 0$, once the components of a cubic elasticity tensor are given (in an arbitrarily oriented basis).

Remark 9.1. To avoid useless computations, it is important to note that, given a cubic elasticity tensor $\mathbf{E} = (\lambda, \mu, 0, 0, \mathbf{H})$, it is equivalent to solve

$$\operatorname{tr}(\mathbf{H} \times \mathbf{a}) = 0, \qquad \mathbf{a} \in \mathbb{H}^2,$$

or to solve

$$\operatorname{tr}(\mathbf{E}^s \times \mathbf{a}) = 0, \qquad \mathbf{a} \in \mathbb{H}^2,$$

where $\mathbf{E}^s$ is the totally symmetric part of $\mathbf{E}$.

The leading harmonic part $\mathbf{H}$ of $\mathbf{E}$ is assumed to be known. Indeed, it has been computed in the previous applications sections for the three optimal tensors $\mathbf{E}^*$, $\mathbf{E}^{**}$ and $\mathbf{F}^{**}$. The methodology to determine the rotation matrix Q is the following.

(1) Compute a basis $(\mathbf{a}_1, \mathbf{a}_2)$ of the two-dimensional space of solutions of the linear system $\mathbf{L}(\mathbf{a}) = 0$.
(2) The pair of second-order tensors $(\mathbf{a}_1, \mathbf{a}_2)$ is orthotropic [53]. Hence, a random tensor $\mathbf{a} = t\mathbf{a}_1 + s\mathbf{a}_2$ in this subspace will be generically orthotropic (as also, almost certainly, both $\mathbf{a}_1$, $\mathbf{a}_2$ computed by a Computer Algebra System). For such an orthotropic tensor, an orthogonal basis of eigenvectors $\boldsymbol{u}_i$ will provide the solution as the rotation matrix $Q = (\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3)$.
(3) The normal form $\mathbf{E}_{\mathbb{O}}$ of $\mathbf{E}$ is then obtained as

$$\mathbf{E}_{\mathbb{O}} = Q \star \mathbf{E}, \qquad (\mathbf{E}_{\mathbb{O}})_{ijkl} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}E_{pqrs}.$$

Rotation associated with the cubic normal form for $\mathbf{E}^*$. Let us first apply this methodology to the cubic tensor $\mathbf{E} = \mathbf{E}^* = (\lambda_0, \mu_0, 0, 0, \mathbf{H} = \mathbf{H}^*)$ the nearest to $\mathbf{E}_0$ (given by (28)). A basis for the space of traceless solutions for the system $\mathbf{L}(\mathbf{a}) = \operatorname{tr}(\mathbf{H}^* \times \mathbf{a}) = 0$ is

$$\mathbf{a}_1 = \begin{pmatrix} 1 & 0.1719141925 & -0.4213723048 \\ 0.1719141925 & -0.3670248470 & 0 \\ -0.4213723048 & 0 & -0.6329751530 \end{pmatrix},$$

$$\mathbf{a}_2 = \begin{pmatrix} 0 & -0.1797028254 & -1.106498932 \\ -0.1797028254 & 3.880108140 & 1 \\ -1.106498932 & 1 & -3.880108140 \end{pmatrix},$$

and the associated eigenvectors matrix Q is

$$Q = \begin{pmatrix} -0.244381988215706 & 0.112674376458757 & -0.963110548548488 \\ -0.966260413618850 & -0.111624674249115 & 0.232122263412857 \\ 0.0813526699553721 & -0.987342097243103 & -0.136151849428213 \end{pmatrix}. \tag{34}$$

Finally, the normal form of $\mathbf{E}^*$ is $\mathbf{E}^*_{\mathbb{O}} = Q \star \mathbf{E}^*$, and one recovers (29).

Rotation associated with the cubic normal forms for $\mathbf{E}^{**}$ and $\mathbf{F}^{**}$. The methodology also applies to the optimal cubic tensors $\mathbf{E}^{**}$ and $\mathbf{F}^{**}$ of section 8 . A basis for the space of traceless solutions for the system $\operatorname{tr}(\mathbf{H}^{**} \times \mathbf{a}) = 0$ is

$$\mathbf{a}_1 = \begin{pmatrix} 1 & 0 & -25.46740405 \\ 0 & 37.84482400 & 20.16410890 \\ -25.46740405 & 20.16410890 & -38.84482400 \end{pmatrix},$$

$$\mathbf{a}_2 = \begin{pmatrix} 0 & 1 & 49.43123622 \\ 1 & -76.54548515 & -40.58449192 \\ 49.43123622 & -40.58449192 & 76.54548515 \end{pmatrix},$$

and the associated eigenvectors matrix Q is

$$Q = \begin{pmatrix} -0.407028622361688 & 0.194165806279755 & -0.892539825582074 \\ 0.167497955759488 & -0.944709963469717 & -0.281899839903180 \\ -0.897926575725844 & -0.264239899698699 & 0.352001619332188 \end{pmatrix}. \tag{35}$$

The normal forms of $\mathbf{E}^{**}$ and $\mathbf{F}^{**}$ are $\mathbf{E}^{**}_{\mathbb{O}} = Q \star \mathbf{E}^{**}$ and $\mathbf{F}^{**}_{\mathbb{O}} = Q \star \mathbf{F}^{**}$. They are (simultaneously) obtained for the (same) rotation Q. One then recovers the normal forms given at the end of section 8 (*i.e.*, in Voigt notation, the matrices $[\mathbf{E}^{**}_{\mathbb{O}}]$ and $[\mathbf{F}^{**}_{\mathbb{O}}]$).

10. Conclusion

Thanks to the recent characterization of the cubic elasticity symmetry classes by polynomial covariants [53], we have formulated the *distance to cubic symmetry problem* as a polynomial optimization problem, and derived the associated Euler–Lagrange equations. We have used the theory of Gröbner bases to solve these equations, in a quasi-analytical manner (using a Computer Algebra System). This methodology has been applied to the case of a single elasticity tensor, as well as to the case of a pair of Hooke and Hill elasto-plasticity tensors. Besides, we have recovered the normal forms of the optimal cubic elasticity/plasticity tensors.

The key-point of the study is that the corresponding cubic symmetry is defined by a polynomial tensorial equation, which is a submersion (apart from the isotropic singularity, which is controlled). This makes it possible to apply the Euler–Lagrange method and use Gröbner bases to compute the critical points.

Appendix A. Solving algebraic systems using Gröbner bases

In this appendix, we propose to explain how to use *Gröbner bases* to solve non-linear algebraic systems. Our goal is not to summarize the theory of Gröbner bases, nor to introduce the basics of algebraic geometry but to explain through some examples how it works. For more details on this topic and a deeper insight, we strongly recommend the following books [19, 60], which contain a lot of references.

Gröbner bases were introduced in the sixties by Buchberger [17]. Like Gaussian elimination method is used to solve a system of linear equations, Gröbner bases are useful to solve a system of non-linear algebraic equations

$$\begin{cases} f_1(x_1,\dots,x_n) & = 0 \\ \dots \\ f_m(x_1,\dots,x_n) & = 0 \end{cases} \tag{36}$$

where $f_1,\dots,f_m$ are polynomial functions in the variables $x_1,\dots,x_n$. Note however that in general, and even for one variable, it is useless to search for closed-form solutions. Therefore, what is expected is a procedure which produces a new system of algebraic equations which is *simpler*. Contrary to Gauss elimination algorithm, where the variables are naturally ordered by the choice of a basis, we need to choose a total order on monomials in order to make the Gröbner bases algorithm to work. There are many total orders on monomials in several variables, the most common being the lexicographic order induced by $x_1 < x_2 < \dots < x_n$, and the resulting Gröbner basis will depend drastically on the choice of an order.

Let us illustrate what we mean here through an example. Consider, for instance, an intersection of three quadrics in $\mathbb{R}^3$, given by the following non-linear system of three homogeneous polynomial equations of degree 2

$$\begin{cases} x_3^2 + x_2^2 + x_1^2 = 1 \\ x_3^2 + x_1x_2 = 1 \\ x_1x_3 + x_1x_2 = 2. \end{cases} \tag{37}$$

in the three variables (x_1, x_2, x_3). The computation of a Gröbner basis for this system (with the lexicographic order induced by $x_1 < x_2 < x_3$) leads to the following equivalent system of equations

$$\begin{cases} 3x_3^8 + 3x_3^6 + 6x_3^4 + 3x_3^2 + 1 = 0 \\ x_2 = -\dfrac{3}{2}x_3^7 - 3x_3^3 + \dfrac{1}{2}x_3 \\ x_1 = -3x_3^7 - 3x_3^5 - 6x_3^3 - 2x_3. \end{cases}$$

Therefore, in this example, computing a Gröbner basis for a system of n equations in n variables leads to an equivalent system of equations of the form

$$\begin{cases} P_n(x_n) = 0 \\ x_{n-1} = P_{n-1}(x_n) \\ \dots \\ x_1 = P_1(x_n) \end{cases} \tag{38}$$

In other words, in that case, one has been able to reduce the non-linear algebraic system (37) to an equivalent triangular system consisting in one polynomial equation in the last variable x_n and a list of $n-1$ equations which are solved in the remaining variables $x_{n-1}, \dots, x_1$. In particular, such a system *has at most a finite number of solutions.*

This is generally what happens if one tries to solve an algebraic system of n equations in n variables but there exists, nevertheless, some *degenerate* situations (as it is the case for linear systems when the determinant of the system vanishes). In the next example, we will illustrate this degeneracy. Consider the following set of equations

$$\begin{cases} x_1^2 + x_2^2 + x_3^2 = 1 \\ x_1 x_2 + x_3^2 = 1 \\ x_2^2 - x_1 x_2 + x_1^2 = 0. \end{cases} \tag{39}$$

An equivalent system given by the computation of a Gröbner basis (for the lexicographic order induced by $x_1 < x_2 < x_3$) is

$$\begin{cases} x_3^2 + x_1 x_2 - 1 = 0 \\ -x_2 x_3^2 + x_1 x_3^2 - x_2^3 + x_2 - x_1 = 0 \\ x_3^4 + x_2^2 x_3^2 - 2x_3^2 + x_2^4 - x_2^2 + 1 = 0 \\ x_3^2 + x_2^2 + x_1^2 - 1 = 0 \end{cases}$$

This time, the explicit solution of the problem is far less straightforward (it will be given and explained anyway below). What we can observe, however, is that the third equation in (39) is a linear combination of the first two ones. Thus, the system is in fact rectangular (two equations in three variables, rather than three equations). More generally, this situation appears for systems of n algebraic equations with n variables each time the polynomials $f_1, \dots, f_n$ are *algebraically dependent.*

Let us discuss now in which way we can interpret this procedure as an extension to systems of polynomial equations of the Gaussian elimination algorithm. In Gauss algorithm, a succession of invertible linear transformations reduces a general system of linear equations into one which is triangular. The first equation involves all the variables, the second equation does not involve x_1, the third equation does not involved x_1, x_2, ... In the nonlinear case a similar process occurs somehow but requires, to be described correctly, to define the notion of *ideal.*

An ideal I of the algebra $\mathbb{C}[x_1, \dots, x_n]$ is a subalgebra of $\mathbb{C}[x_1, \dots, x_n]$ which is stable by multiplication by every polynomial in $\mathbb{C}[x_1, \dots, x_n]$. More precisely, this means that

$$f \in I \quad \text{and} \quad p \in \mathbb{C}[x_1, \dots, x_n] \implies pf \in I.$$

Now consider the system (36) and the ideal

$$I := \{p_1 f_1 + \dots + p_m f_m;\ p_k \in \mathbb{C}[x_1, \dots, x_n]\},$$

generated by $f_1, \dots, f_m$. It is clear that every $f \in I$ vanishes on each solution of (36), and conversely that the solutions of (36) can be recast as the solutions of the infinite system of equations

$$f(x_1, \dots, x_n) = 0, \qquad f \in I.$$

Now, let us introduce the l-th *elimination ideal*

$$I_l := I \cap \mathbb{C}[x_{l+1}, \dots, x_n], \qquad l = 1, \dots, n-1.$$

Note that I_l is an ideal of $\mathbb{C}[x_{l+1},\dots,x_n]$ but not of $\mathbb{C}[x_1,\dots,x_n]$. It is however a subalgebra of $\mathbb{C}[x_1,\dots,x_n]$ and we have

$$I_{n-1}\subset\cdots\subset I_1\subset I.$$

Then, a Gröbner basis (computed using the lexicographic order induced by $x_1<x_2<\cdots<x_n$) provides a new system of generators of I which is compatible with the sequence of elimination ideals. Let us illustrate what we mean here, using our first example (37). In that case, the following Gröbner basis was computed

$$\begin{cases} g_1=-3x_3^7-3x_3^5-6x_3^3-2x_3-x_1,\\ g_2=3x_3^7+6x_3^3-x_3+2x_2,\\ g_3=-3x_3^8-3x_3^6-6x_3^4-3x_3^2-1.\end{cases}$$

In this example, I is generated by g_1,g_2,g_3, I_1 by g_2,g_3 and I_2 by g_3. It is in this sense that a Gröbner basis can be considered as a *triangulation* of the initial problem. Hence, in this example, solving the problem consists first in finding the roots of $g_3=0$, then calculating x_2 using $g_2=0$ and then x_1 using $g_1=0$. Consider now the second example (39). In that case, the following Gröbner basis was computed using the lexicographic order $x_1<x_2<x_3$

$$\begin{cases} g_1=x_3^2+x_1x_2-1,\\ g_2=-x_2x_3^2+x_1x_3^2-x_2^3+x_2-x_1,\\ g_3=x_3^2+x_2^2+x_1^2-1,\\ g_4=x_3^4+x_2^2x_3^2-2x_3^2+x_2^4-x_2^2+1.\end{cases}$$

In this example, I is generated by g_1,g_2,g_3,g_4, I_1 by g_4 and I_2 by 0. We could continue here to explain the complete resolution of the problem but it appears that changing the order on monomials makes the resolution by far much more readable for a human being. Indeed, changing the lexicographic order $x_1<x_2<x_3$ to $x_3<x_1<x_2$ leads to the following Gröbner basis

$$\begin{cases} g_1=x_3^2-1+x_1x_2,\\ g_2=x_1^2-x_1x_2+x_2^2,\end{cases}$$

and, then, I is generated by g_1,g_2, $I_1:=I\cap\mathbb{C}[x_1,x_2]$ by g_2 and $I_2:=I\cap\mathbb{C}[x_2]$ by 0. We will now proceed to the complete resolution of the system. First, we need to solve the equation in one variable x_2 given by I_2. Since I_2 is generated by 0, this means that the variable x_2 is free. We will thus set $x_2=t$ ($t\in\mathbb{C}$). Then, we need to solve the system of equations in two variables (x_2,x_1) given by I_1. More precisely, since we have already solved the problem for x_2 (the system is triangular), we seek solutions (x_2,x_1) of

$$x_1^2-x_1x_2+x_2^2=0,$$

which *extend* the solution $x_2=t$. Hence, x_2 is no more a variable here but a parameter. This equation has either one solution $(x_2=0,x_1=0)$ if $t=0$ or two conjugate imaginary solutions if $t\neq 0$. Now, we need to solve the system of equations in three variables (x_2,x_1,x_3) given by I. Hence, we need to solve the equation

$$x_3^2-1+x_1x_2=0$$

but where $(x_2=a,x_1=b)$ is a solution of the previous step and where $x_2=a$ and $x_1=b$ should be considered as parameters of the problem. Such a solution is said *to extend* the previous one. In our example, we find exactly two solutions for x_3 for each solution $(x_2=a,x_1=b)$ (because the coefficient of x_3^2 is one). In other examples, nevertheless, some solutions could be *not extendable* (for example, if the coefficient of x_3^2 depends on a, b and vanishes for some values of a and b). This example illustrate the *triangular process* allowed by the computation of a Gröbner basis in solving non-linear algebraic equations. Note finally that solutions are sought in $\mathbb{C}$. In this example, there are an infinite number of complex solutions. Of course, it may happen that there are no real solution at all.

Remark A.1. The Gröbner bases are exact when computed over the field $\mathbb{Q}$ of rational numbers. It is a natural question whether or not, one could work with Groebner bases with coefficients in the field of real or complex numbers, or to be more exact, using floating numbers. In practice, this is a difficult topic since there are convergence/accuracy issues. Anyway, this subject is a research area called *Groebner bases with coefficients in an inexact field.* We redirect the interested reader to [49].

Appendix B. Upper bounds estimates of the distance to cubic elasticity

Baerheim [11] has observed that the dilatation tensor $\mathbf{d}_0 = \mathrm{tr}_{12}\,\mathbf{E}_0$, and the Voigt tensor $\mathbf{v}_0 = \mathrm{tr}_{13}\,\mathbf{E}_0$, both second-order covariants of $\mathbf{E}_0$, generically carry information related to a "natural" basis of an elasticity tensor. Using accordingly an eigenbasis of

$$\mathbf{t}_0 = \mathbf{A}_0 : \mathbf{1} - \frac{1}{4}(\mathbf{1} : \mathbf{A}_0 : \mathbf{1})\,\mathbf{1}, \quad \text{such as} \quad \mathbf{t}_0' = \frac{2}{3}\left(\mathbf{d}_0' - \mathbf{v}_0'\right),$$

built from the asymmetric part $\mathbf{A}_0 = \mathbf{E}_0 - (\mathbf{E}_0)^s$ (in the sense of Backus [10]) of the raw/measured elasticity tensor, Stahn and coworkers astutely define an upper bound estimate $M(\mathbf{E}_0, [G])$ of the distance to a 3D elasticity symmetry class $[G]$, in a few steps [59]:

(1) by computing an eigenbasis of $\mathbf{t}_0$ and a rotation Q_0 that brings it into its diagonal form (*i.e.*, such that $Q_0 \star \mathbf{t}_0 = Q_0\,\mathbf{t}_0\,Q_0^T$ and $Q_0 \star \mathbf{t}_0'$ are diagonal),
(2) by computing $Q_0 \star \mathbf{E}_0$,
(3) finally, by setting

$$M(\mathbf{E}_0, [G]) := \min_{Q \in \mathbb{O}} \|Q \star Q_0 \star \mathbf{E}_0 - \mathbf{R}_G\,(Q \star Q_0 \star \mathbf{E}_0)\|, \tag{40}$$

with the property $Q \star Q_0 \star \mathbf{E}_0 = (QQ_0) \star \mathbf{E}_0$ and where $\mathbf{R}_G$ is the Reynolds operator (an orthogonal projector [60, Chapter 2], see also [6, Appendix C]), associated with the group G representative of the considered symmetry class.

In particular, for the cubic elasticity case and the finite proper octahedral (cubic) group $G = \mathbb{O}$ (of order 24), one has

$$\mathbf{R}_{\mathbb{O}}\,(\mathbf{E}) = \frac{1}{24}\sum_{i=1}^{24} R_i \star \mathbf{E},$$

where the rotations $R_1 = \mathrm{I}, R_2, \ldots, R_{24}$ are the 24 elements of the group $\mathbb{O}$.

Remark B.1. The definition (40) does not depend on a particular choice of the rotation Q_0, among the 24 possibilities bringing $\mathbf{t}_0$ into its diagonal form.

It is here important to point out that difficulties arise for cubic symmetry as the second-order covariants $\mathbf{c}(\mathbf{E})$ of a cubic tensor $\mathbf{E}$ (such as $Q \star \mathbf{c}(\mathbf{E}) = \mathbf{c}(Q \star \mathbf{E})\ \forall Q \in \mathrm{SO}(3)$) are all isotropic, *i.e.* spherical. Indeed, they inherit the cubic symmetry group of $\mathbf{E}$, and a cubic second-order order tensor is necessarily isotropic. This point is discussed in [11, 52, 2, 59]. For a material with a close to be cubic microstructure, it is expected that, even if the measured tensor $\mathbf{t}_0$ is orthotropic, the related eigenbasis information may be not relevant and may be of the order of magnitude of the measurement noise.

This is why, starting from the harmonic decomposition of a given triclinic elasticity tensor

$$\mathbf{E}_0 = (\lambda_0, \mu_0, \mathbf{d}_0', \mathbf{v}_0', \mathbf{H}_0),$$

we propose another upper bound estimate of the distance of $\mathbf{E}_0$ to elasticity cubic symmetry, as

$$\Delta(\mathbf{E}_0, [\mathbb{O}]) := \|\mathbf{E}_0 - \mathbf{E}^{\mathrm{upper}}\|, \tag{41}$$

where the cubic elasticity tensor

$$\mathbf{E}^{\mathrm{upper}} := 2\mu_0\mathbf{I} + \lambda_0\mathbf{1} \otimes \mathbf{1} + (\mathbf{C}_0 :: \mathbf{H}_0)\,\mathbf{C}_0 \tag{42}$$

is computed from the cubic harmonic fourth-order tensor of unit norm

$$\mathbf{C}_0 := \sqrt{\frac{15}{2}}\,\frac{\left[\left(\mathbf{d}_2^2 \times \mathbf{d}_2\right) \cdot \left(\mathbf{d}_2^2 \times \mathbf{d}_2\right)\right]'}{\|\mathbf{d}_2^2 \times \mathbf{d}_2\|^2}, \quad \text{with} \quad \mathbf{d}_2 = \mathbf{H}_0 \,\vdots\, \mathbf{H}_0,$$

$(\cdot)'$ denoting the harmonic fourth-order part. Both $\mathbf{E}^{\text{upper}}$ and $\Delta(\mathbf{E}_0, [\mathbb{O}])$ are thus built from a cubic fourth-order covariant ($\mathbf{C}_0$) defined from the fourth-order harmonic part $\mathbf{H}_0$ of the raw tensor $\mathbf{E}_0$ ($\mathbf{C}_0$ is naively assumed to better carry the cubic basis than $\mathbf{d}_0$, $\mathbf{v}_0$ or $\mathbf{t}_0$).

Component formulas for the generalized cross product $\mathbf{d}_2^2 \times \mathbf{d}_2$ (a third order tensor defined by (3)) are given in [2, Appendix B]. Note that

$$\|\mathbf{d}_2^2 \times \mathbf{d}_2\|^2 = \frac{1}{12}\left(\left(\operatorname{tr}(\mathbf{d}_2'^2)\right)^3 - 6\left(\operatorname{tr}(\mathbf{d}_2'^3)\right)^2\right).$$

and

$$\left[\left(\mathbf{d}_2^2 \times \mathbf{d}_2\right) \cdot \left(\mathbf{d}_2^2 \times \mathbf{d}_2\right)\right]' = \left(\mathbf{d}_2^2 \times \mathbf{d}_2\right) \cdot \left(\mathbf{d}_2^2 \times \mathbf{d}_2\right) - \frac{1}{15}\|\mathbf{d}_2^2 \times \mathbf{d}_2\|^2 \left(3\,\mathbf{I} - \mathbf{1} \otimes \mathbf{1}\right).$$

Remark B.2. The fourth order tensor $\mathbf{C}_0$ is a rational covariant of $\mathbf{H}_0$, therefore of $\mathbf{E}_0$. It is built from the second-order quadratic covariant $\mathbf{d}_2 = \mathbf{d}_2(\mathbf{E}_0)$. When $\mathbf{d}_2$ is orthotropic (which is generically the case for the raw/measured tensor $\mathbf{E}_0$) the third-order tensor $\mathbf{d}_2^2 \times \mathbf{d}_2$ is tetrahedral and harmonic, and the fourth-order tensor $(\mathbf{d}_2^2 \times \mathbf{d}_2) \cdot (\mathbf{d}_2^2 \times \mathbf{d}_2)$ is cubic but not harmonic [51].

Using (18), an invariant formula for the upper bound estimate (41)–(42) is finally

$$\Delta(\mathbf{E}_0, [\mathbb{O}]) = \sqrt{\frac{2}{21}\|\mathbf{d}_0' + 2\mathbf{v}_0'\|^2 + \frac{4}{3}\|\mathbf{d}_0' - \mathbf{v}_0'\|^2 + \|\mathbf{H}_0\|^2 - (\mathbf{C}_0 :: \mathbf{H}_0)^2}\ . \tag{43}$$

The upper bound estimates (40) and (43) as well as the relative estimates

$$\frac{M(\mathbf{E}_0, [\mathbb{O}])}{\|\mathbf{E}_0\|} \quad \text{and} \quad \frac{\Delta(\mathbf{E}_0, [\mathbb{O}])}{\|\mathbf{E}_0\|}$$

are compared in Table 1 with the exact distance $d(\mathbf{E}_0, \text{cubic symmetry})$ and with the relative distance $d(\mathbf{E}_0, \text{cubic symmetry})/\|\mathbf{E}_0\|$ computed in section 6 for the raw elasticity tensor (26). The upper bounds estimates are found not very accurate, the proposed upper bound estimate $\Delta(\mathbf{E}_0, [\mathbb{O}])$ (built from $\mathbf{H}_0$) being only slightly better than the estimate $M(\mathbf{E}_0, [\mathbb{O}])$ (built from $\mathbf{d}_0' - \mathbf{v}_0'$)). This shows the difficulty to define an accurate estimate of the distance to cubic elasticity from second-order covariants of the raw elasticity tensor, and underlines the interest of being able to compute the exact distance $d(\mathbf{E}_0, \text{cubic symmetry})$.

	$d(\mathbf{E}_0, \text{cubic symmetry})$	$M(\mathbf{E}_0, [\mathbb{O}])$	$\Delta(\mathbf{E}_0, [\mathbb{O}])$
Distance/estimates (GPa)	74.13	245.5	238.6
Relative distance/estimates	0.1039	0.3441	0.3344

TABLE 1. Comparison of upper bounds estimates of the distance to cubic elasticity.

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Appendix A

Normal form of the coupled Piezoelectricity law

Consider the representation of the rotation group (SO(3) or O(3)) on the space of tensors (see chapter 3). A material is not represented by a unique tensor $\mathbf{T}$ but by the orbit of $\mathbf{T}$. Among the tensors that belong to the orbit of $\mathbf{T}$, there exists one tensor that is fixed by all the rotations of the symmetry group of $\mathbf{T}$, this tensor is called the *normal form* of $\mathbf{T}$. In other words, the normal form of a tensor $\mathbf{T}$, having the symmetry of a subgroup H of G, is an element of the fixed point set defined as follows

$$\mathbb{F}\mathrm{ix}(H) = \{\mathbf{T} \ \mid \ \forall g \in H, \ g \star \mathbf{T} = \mathbf{T}\}.$$

The orthonormal basis in which the normal form of a tensor $\mathbf{T}$ is represented is called *natural basis* for $\mathbf{T}$. Every tensor $\mathbf{T}$ having a symmetry group H can be expressed in its normal form. In fact, one can deduce the symmetry of a tensor if it is given in its natural basis.

Consider the representation of O(3) on the space of Piezoelectricity constitutive tensors for the coupled law described in chapter 4 (see (4.1)). A normal form of a triplet $\mathcal{P} \in \mathcal{P}\mathrm{iez}$, having the symmetry of a subgroup H, is a triplet of tensors that are fixed by all the elements of H. In other terms, a normal form of $\mathcal{P} \in \mathcal{P}\mathrm{iez}$ for the subgrup H belongs to the fixed-point set

$$\mathbb{F}\mathrm{ix}(H) = \{\mathcal{P} = (\mathbf{E}, \mathbf{P}, \mathbf{S}) \in \mathcal{P}\mathrm{iez} \ \mid \ \forall h \in H, (\rho(h)\mathbf{E}, \rho(h)\mathbf{P}, \rho(h)\mathbf{S}) = (\mathbf{E}, \mathbf{P}, \mathbf{S})\}$$

where (see chapter 4)

$$(\rho(h)\mathbf{E})_{ijkl} = g_{ip}g_{jq}g_{kr}g_{ls}E_{pqrs}, \quad (\rho(h)\mathbf{P})_{ijk} = g_{ip}g_{jq}g_{kr}P_{pqr}, \quad (\rho(h)\mathbf{S})_{ij} = g_{ip}g_{jq}S_{pq}.$$

In this part, a basis of the fixed-point set of each isotropy class of the coupled law $\mathcal{P}\mathrm{iez}$, given in theorem 4.4.1, is computed. We used [53, theorem 3.2 and theorem 3.5] to calculate the dimension of each fixed-point set given in tables A.1, A.2 and A.3.

$[H]$	$[\mathbb{1}]$	$[\mathbb{Z}_2]$	$[\mathbb{Z}_3]$	$[\mathbb{Z}_4]$	$[\mathbb{D}_2]$	$[\mathbb{D}_3]$	$[\mathbb{D}_4]$	$[\mathrm{SO}(2)]$	$[\mathrm{O}(2)]$	$[\mathrm{O}(3)]$
$\dim(\mathbb{F}\mathrm{ix}(H))$	45	25	15	13	15	10	9	11	8	0

Table A.1: Dimension of the fixed-point sets for each symmetry class of $\mathcal{P}$iez of type I

$[H]$	$[\mathbb{Z}_2 \oplus \mathbb{Z}_2^c]$	$[\mathbb{D}_2 \oplus \mathbb{Z}_2^c]$	$[\mathbb{D}_3 \oplus \mathbb{Z}_2^c]$	$[\mathbb{D}_4 \oplus \mathbb{Z}_2^c]$	$[\mathbb{O} \oplus \mathbb{Z}_2^c]$	$[\mathrm{O}(2) \oplus \mathbb{Z}_2^c]$
$\dim(\mathbb{F}\mathrm{ix}(H))$	17	12	8	8	4	7

Table A.2: Dimension of the fixed-point sets for each symmetry class of $\mathcal{P}$iez of type II

$[H]$	$[\mathbb{Z}_2^-]$	$[\mathbb{Z}_4^-]$	$[\mathbb{Z}_6^-]$	$[\mathbb{D}_2^z]$	$[\mathbb{D}_3^z]$	$[\mathbb{D}_4^z]$	$[\mathbb{D}_2^d]$	$[\mathbb{D}_4^d]$	$[\mathbb{D}_6^d]$	$[\mathbb{O}^-]$	$[\mathrm{O}(2)^-]$
$\dim(\mathbb{F}\mathrm{ix}(H))$	27	13	9	17	12	11	17	10	8	5	10

Table A.3: Dimension of the fixed-point sets for each symmetry class of $\mathcal{P}$iez of type III

Let $(\mathbf{E}, \mathbf{P}, \mathbf{S}) \in \mathcal{P}$iez, $\mathbf{E}, \mathbf{P}$ and $\mathbf{S}$ can be represented by the following matrices (in Voigt notation):

$$[\mathbf{E}] = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & E_{1123} & E_{1131} & E_{1112} \\ E_{1122} & E_{2222} & E_{2233} & E_{2223} & E_{2231} & E_{2212} \\ E_{1133} & E_{2233} & E_{3333} & E_{3323} & E_{3331} & E_{3312} \\ E_{1123} & E_{2223} & E_{3323} & E_{2323} & E_{2331} & E_{2312} \\ E_{1131} & E_{2231} & E_{3331} & E_{2331} & E_{1313} & E_{3112} \\ E_{1112} & E_{2212} & E_{3312} & E_{2312} & E_{3112} & E_{1212} \end{pmatrix},$$

$$[\mathbf{P}] = \begin{pmatrix} P_{111} & P_{122} & P_{133} & P_{123} & P_{113} & P_{112} \\ P_{211} & P_{222} & P_{233} & P_{223} & P_{213} & P_{212} \\ P_{311} & P_{322} & P_{333} & P_{323} & P_{313} & P_{312} \end{pmatrix} \text{ and } [\mathbf{S}] = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{12} & S_{22} & S_{23} \\ S_{13} & S_{23} & S_{33} \end{pmatrix}$$

A basis of the fixed-point set of a subgroup H is computed by solving a linear system defined using the generators of H from table 3.1: if h_i are the generators of H then we have

$$\begin{cases} \rho(h_i)\mathbf{E} = \mathbf{E} & \forall i \\ \rho(h_i)\mathbf{P} = \mathbf{P} & \forall i \\ \rho(h_i)\mathbf{S} = \mathbf{S} & \forall i \end{cases}$$

In the following, an element of each fixed-point set is represented by a triplet of normal forms in their matrix representation. A triplet of $\mathbb{F}\mathrm{ix}(H)$ is denoted by $[N]_H = ([\mathbf{E}]_H, [\mathbf{P}]_H, [\mathbf{S}]_H)$.

A.0.1 Symmetry classes of type I

$$[N]_{\mathbb{Z}_2} = \left(\begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & E_{1112} \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & E_{2212} \\ E_{1133} & E_{2233} & E_{3333} & 0 & 0 & E_{3312} \\ 0 & 0 & 0 & E_{2323} & E_{2331} & 0 \\ 0 & 0 & 0 & E_{2331} & E_{1313} & 0 \\ E_{1112} & E_{2212} & E_{3312} & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & P_{123} & P_{113} & 0 \\ 0 & 0 & 0 & P_{223} & P_{213} & 0 \\ P_{311} & P_{322} & P_{333} & 0 & 0 & P_{312} \end{pmatrix}, \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{12} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathbb{Z}_3} = \left(\left(\begin{pmatrix} E_{2222} & -2E_{1212}+E_{2222} & E_{2233} & E_{3112} & -E_{2312} & 0 \\ -2E_{1212}+E_{2222} & E_{2222} & E_{2233} & -E_{3112} & E_{2312} & 0 \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ E_{3112} & -E_{3112} & 0 & E_{2323} & 0 & E_{2312} \\ -E_{2312} & E_{2312} & 0 & 0 & E_{2323} & E_{3112} \\ 0 & 0 & 0 & E_{2312} & E_{3112} & E_{1212} \end{pmatrix}, \right.\right.$$
$$\left.\left. \begin{pmatrix} -P_{212} & P_{212} & 0 & -P_{213} & P_{223} & -P_{222} \\ -P_{222} & P_{222} & 0 & P_{223} & P_{213} & P_{212} \\ P_{322} & P_{322} & P_{333} & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right) \right)$$

$$[N]_{\mathbb{Z}_4} = \left(\begin{pmatrix} E_{2222} & E_{1122} & E_{2233} & 0 & 0 & -E_{2212} \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & E_{2212} \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ -E_{2212} & E_{2212} & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & -P_{213} & P_{223} & 0 \\ 0 & 0 & 0 & P_{223} & P_{213} & 0 \\ P_{322} & P_{322} & P_{333} & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathbb{D}_2} = \left(\begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & 0 \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{1133} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & P_{123} & 0 & 0 \\ 0 & 0 & 0 & 0 & P_{213} & 0 \\ 0 & 0 & 0 & 0 & 0 & P_{312} \end{pmatrix}, \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathbb{D}_3} = \left(\left(\begin{pmatrix} E_{2222} & -2E_{1212}+E_{2222} & E_{2233} & E_{3112} & 0 & 0 \\ -2E_{1212}+E_{2222} & E_{2222} & E_{2233} & -E_{3112} & 0 & 0 \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ E_{3112} & -E_{3112} & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & E_{3112} \\ 0 & 0 & 0 & 0 & E_{3112} & E_{1212} \end{pmatrix}, \right.\right.$$
$$\left.\left. \begin{pmatrix} -P_{212} & P_{212} & 0 & -P_{213} & 0 & 0 \\ 0 & 0 & 0 & 0 & P_{213} & P_{212} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right) \right)$$

$$[N]_{\mathbb{D}_4} = \left(\begin{pmatrix} E_{2222} & E_{1122} & E_{2233} & 0 & 0 & 0 \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & -P_{213} & 0 & 0 \\ 0 & 0 & 0 & 0 & P_{213} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathrm{SO}(2)} = \left(\begin{pmatrix} E_{2222} & -2E_{1212}+E_{2222} & E_{1133} & 0 & 0 & 0 \\ -2E_{1212}+E_{2222} & E_{2222} & E_{1133} & 0 & 0 & 0 \\ E_{1133} & E_{1133} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1313} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} 0 & 0 & 0 & -P_{213} & P_{113} & 0 \\ 0 & 0 & 0 & P_{113} & P_{213} & 0 \\ P_{311} & P_{311} & P_{333} & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathrm{O}(2)} = \left(\begin{pmatrix} E_{2222} & -2E_{1212}+E_{2222} & E_{1133} & 0 & 0 & 0 \\ -2E_{1212}+E_{2222} & E_{2222} & E_{1133} & 0 & 0 & 0 \\ E_{1133} & E_{1133} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1313} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} 0 & 0 & 0 & -P_{213} & 0 & 0 \\ 0 & 0 & 0 & 0 & P_{213} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right).$$

A.0.2 Symmetry classes of type II

The normal form of a $\mathcal{P}$iez tensor belonging to a symmetry class of type II can be deduced from the previous subsection using the following lemma.

Lemma A.0.1. *Let H be a subgroup of type I. We have*

$$\mathbb{F}\mathrm{ix}_{\mathcal{P}iez}(H \oplus \mathbb{Z}_2^c) = \mathbb{F}\mathrm{ix}_{\mathbb{E}\mathrm{la}\oplus\mathbb{S}}(H).$$

Proof. The result follows using the harmonic decomposition of $\mathcal{P}$iez (deduced from the harmonic decomposition of $\mathbb{P}$iez ([89]), $\mathbb{E}$la and $\mathbb{S}$ ([90]))

$$\mathcal{P}\mathrm{iez} = \mathbb{H}^4 \oplus \mathbb{H}^3 \oplus 3\mathbb{H}^2 \oplus \mathbb{H}^{-2} \oplus 2\mathbb{H}^1 \oplus 3\mathbb{H}^0,$$

and the following two assertions:

1. Let G be a group and (V, ρ) be a linear representation such that $V = V_1 \oplus V_2$ stable. Then for all H subgroup of G

$$\mathbb{F}\mathrm{ix}_V(H) = \mathbb{F}\mathrm{ix}_{V_1}(H) \oplus \mathbb{F}\mathrm{ix}_{V_2}(H).$$

2. $\mathbb{F}\mathrm{ix}_{\mathbb{H}^n}(H \oplus \mathbb{Z}_2^c) = \begin{cases} \mathbb{F}\mathrm{ix}(H) & \text{if } n \text{ is even } (\rho(-\mathrm{I}) = \mathrm{I}) \\ 0 & \text{if } n \text{ is odd } (\rho(-\mathrm{I}) = -\mathrm{I}) \end{cases}.$

Hence, we have $\mathbb{F}\mathrm{ix}_{\mathcal{P}\mathrm{iez}}(H \oplus \mathbb{Z}_2^c) = \mathbb{F}\mathrm{ix}_{\mathbb{H}^4\oplus 3\mathbb{H}^2\oplus 3\mathbb{H}^0}(H) = \mathbb{F}\mathrm{ix}_{\mathbb{E}\mathrm{la}\oplus\mathbb{S}}(H)$. □

We can deduce from the previous lemma that

$$[\mathbf{E}]_{H\oplus\mathbb{Z}_2^c} = [\mathbf{E}]_H,\ [\mathbf{P}]_{H\oplus\mathbb{Z}_2^c} = 0 \text{ and } [\mathbf{S}]_{H\oplus\mathbb{Z}_2^c} = [\mathbf{S}]_H.$$

A.0.3 Symmetry classes of type III

$$[N]_{\mathbb{Z}_2^-} = \left(\begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & E_{1112} \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & E_{2212} \\ E_{1133} & E_{2233} & E_{3333} & 0 & 0 & E_{3312} \\ 0 & 0 & 0 & E_{2323} & E_{2331} & 0 \\ 0 & 0 & 0 & E_{2331} & E_{1313} & 0 \\ E_{1112} & E_{2212} & E_{3312} & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} P_{111} & P_{122} & P_{133} & 0 & 0 & P_{112} \\ P_{211} & P_{222} & P_{233} & 0 & 0 & P_{212} \\ 0 & 0 & 0 & P_{323} & P_{313} & 0 \end{pmatrix}, \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{12} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}\right)$$

$$[N]_{\mathbb{Z}_4^-} = \left(\begin{pmatrix} E_{2222} & E_{1122} & E_{2233} & 0 & 0 & -E_{2212} \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & E_{2212} \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ -E_{2212} & E_{2212} & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} 0 & 0 & 0 & P_{213} & -P_{223} & 0 \\ 0 & 0 & 0 & P_{223} & P_{213} & 0 \\ -P_{322} & P_{322} & 0 & 0 & 0 & P_{312} \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}\right)$$

$$[N]_{\mathbb{Z}_6^-} = \left(\begin{pmatrix} E_{2222} & -2E_{1212}+E_{2222} & E_{2233} & 0 & 0 & 0 \\ -2E_{1212}+E_{2222} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} -P_{212} & P_{212} & 0 & 0 & 0 & -P_{222} \\ -P_{222} & P_{222} & 0 & 0 & 0 & P_{212} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}\right)$$

$$[N]_{\mathbb{D}_2^z} = \left(\begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & 0 \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{1133} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 & P_{113} & 0 \\ 0 & 0 & 0 & P_{223} & 0 & 0 \\ P_{311} & P_{322} & P_{333} & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}\right)$$

$$[N]_{\mathbb{D}_3^z} = \left(\begin{pmatrix} E_{2222} & -2E_{1212}+E_{2222} & E_{2233} & E_{3112} & 0 & 0 \\ -2E_{1212}+E_{2222} & E_{2222} & E_{2233} & -E_{3112} & 0 & 0 \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ E_{3112} & -E_{3112} & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & E_{3112} \\ 0 & 0 & 0 & 0 & E_{3112} & E_{1212} \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} 0 & 0 & 0 & 0 & P_{223} & -P_{222} \\ -P_{222} & P_{223} & 0 & P_{223} & 0 & 0 \\ P_{322} & P_{322} & P_{333} & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}\right)$$

$$[N]_{\mathbb{D}_4^z} = \left(\begin{pmatrix} E_{2222} & E_{1122} & E_{2233} & 0 & 0 & 0 \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 & P_{223} & 0 \\ 0 & 0 & 0 & P_{223} & 0 & 0 \\ P_{322} & P_{322} & P_{333} & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathbb{D}_2^d} = \left(\begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & 0 & 0 & 0 \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{1133} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} P_{111} & P_{122} & P_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & P_{212} \\ 0 & 0 & 0 & 0 & P_{313} & 0 \end{pmatrix}, \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathbb{D}_4^d} = \left(\begin{pmatrix} E_{2222} & E_{1122} & E_{2233} & 0 & 0 & 0 \\ E_{1122} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & P_{213} & 0 & 0 \\ 0 & 0 & 0 & 0 & P_{213} & 0 \\ 0 & 0 & 0 & 0 & 0 & P_{312} \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathbb{D}_6^d} = \left(\begin{pmatrix} E_{2222} & -2E_{1212}+E_{2222} & E_{2233} & 0 & 0 & 0 \\ -2E_{1212}+E_{2222} & E_{2222} & E_{2233} & 0 & 0 & 0 \\ E_{2233} & E_{2233} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{2323} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} -P_{212} & P_{212} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & P_{212} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{22} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathbb{O}^-} = \left(\begin{pmatrix} E_{2222} & E_{1133} & E_{1133} & 0 & 0 & 0 \\ E_{1133} & E_{2222} & E_{1133} & 0 & 0 & 0 \\ E_{1133} & E_{1133} & E_{2222} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1313} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1313} \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & P_{312} & 0 & 0 \\ 0 & 0 & 0 & 0 & P_{312} & 0 \\ 0 & 0 & 0 & 0 & 0 & P_{312} \end{pmatrix}, \begin{pmatrix} S_{33} & 0 & 0 \\ 0 & S_{33} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right)$$

$$[N]_{\mathrm{O}(2)^-} = \left(\begin{pmatrix} E_{2222} & -2E_{1212}+E_{2222} & E_{1133} & 0 & 0 & 0 \\ -2E_{1212}+E_{2222} & E_{2222} & E_{1133} & 0 & 0 & 0 \\ E_{1133} & E_{1133} & E_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{1313} & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{1212} \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} 0 & 0 & 0 & 0 & P_{113} & 0 \\ 0 & 0 & 0 & P_{113} & 0 & 0 \\ P_{311} & P_{311} & P_{333} & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix} \right).$$

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