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Homogeneity without uniformity: towards a mathematical theory of functionally graded materials

Marcelo Epstein^a, Manuel de León^{b,*}

^a Department of Mechanical and Manufacturing Engineering, The University of Calgary, Calgary, Alberta., Canada T2N 1N4

^b Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 123, 28006 Madrid, Spain

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Abstract

Several natural geometric structures are defined that can be associated with material bodies not necessarily possessing the uniformity property, such as functionally graded materials (FGMs). By demanding that only different points have the same type of material symmetry, conditions are derived for the definition of some kind of homogeneity. © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

It is generally known that a uniform elastic body (Noll, 1967) is rich in geometric structure, a fact that has been successfully exploited to model continuous distributions of dislocations and other defects, thermal stresses, and residual stresses in general (Kondo, 1955; Billby, 1960; Kröner, 1960; Noll, 1967; Wang, 1967). It has been shown (Elzanowski et al., 1990) that the basic differential-geometric object involved in this description is a G -structure, whose structural group is the symmetry group of the material and whose integrability corresponds to the physical notion of homogeneity. Extensions of the theory to materials with internal structure (Epstein and de León, 1996, 1998) have brought into play higher order G -structures, but have left the main concepts unchanged. Moreover, some anelastic evolutive phenomena, such as plasticity and growth, can be seen (Epstein and Maugin, 1996, 1998) as precisely defined evolutions of the underlying G -structure within a larger conjugate class.

Roughly speaking, a uniform body is made of the same material at all its points. Homogeneity means that the body can be smoothly deformed so as to bring it to a homogeneous state, namely, a (global)

* Corresponding author. Fax: +1-34-91-5854894.

E-mail addresses: epstein@cnme.ucalgary.ca (M. Epstein), mdeleon@fresno.csic.es (M. de León).

configuration such that all the points “look” exactly the same, as far as their constitutive relations are concerned (for instance, they are all stress free and equally oriented). In the theory of inhomogeneities (Noll, 1967), the uniformity property plays a central role and is, in fact, exploited from the very beginning to yield the notion of material isomorphism for every pair of points in the body. These material isomorphisms generate (local) distant parallelisms, whose integrability measures their ability of becoming straightened, as it were, into a homogeneous configuration. It would appear, therefore, that uniformity is a precondition of homogeneity.

Motivated by the existence of the so-called functionally graded materials (FGMs) (Yamanouchi et al., 1990; Ilshner and Cherradi, 1995; Sánchez Herencia, 1996; Suresh and Mortensen, 1998) which are intrinsically non-uniform, this article addresses the question: can a non-uniform body be considered homogeneous and, if so, what is the underlying geometric object representing this property? It will be shown that if a non-uniform body satisfies the weaker condition of having the same type of material symmetries at every point, there already exists enough structure to define some kind of homogeneity. Moreover, if the material points recognize a preferred state (specifically, the case of elastic solids), then the new notion of homogeneity can be strengthened so as to resemble the conventional one.

The concept of FGMs was first proposed in 1984 as a response to the need for materials which could serve as thermal barriers while developing low residual stresses. Another common application of FGMs is in the field of electroceramics, as actuators and carriers of energy conservation devices. In optics, FGMs can be used to produce fibers with a smoothly varying refractive index. The main idea behind FGMs consists of producing a composite material whose composition varies gradually with position in the body. Thus, FGMs are tailor-made materials developed to suit a variety of particular applications. The methods of fabrication are, correspondingly, very diverse, and new methods are constantly proposed.

Although the mathematics needed to fully appreciate the finer points of the theory is far from elementary, this presentation contains few formulas or manipulations, the emphasis being placed on the seminal ideas. An appendix contains relevant results from the theory of groups, some of which, although elementary, are not easily found in textbooks.

2. Uniformity and homogeneity

The original theory of inhomogeneities within a purely continuum mechanical context is due to Noll (1967) and Wang (1967). This is not to say that these authors were the first to consider continuous distributions of inhomogeneities. Indeed, the works of Kondo (1955), Bilby (1960), Kröner (1960) and others had already demonstrated the need for the use of highly sophisticated differential-geometric tools to represent various possible limiting situations of a defective crystalline lattice. The novelty of Noll's work resides in a derivation of a differential-geometric context only on the basis of the properties of the macroscopic constitutive equation of the body. By not appealing to the presumed knowledge of an underlying atomic lattice, whose imperfections somehow tend to a density, Noll's viewpoint becomes applicable to a wider class of situations, such as those resulting from residual stresses of a general nature even if the lattice is regular or non-existent. Examples of the first situation are provided by thermal stresses and by the forming of a metal ring out of a homogeneous plane strip. Examples of the second type are non-crystalline materials. It should be pointed out that there are other ways to model inhomogeneities (Edelen and Lagoudas, 1988).

Naturally, in the strictly continuum viewpoint, the definition of inhomogeneity density can no longer be based upon a heuristic passage to the limit of a defective lattice as the interatomic distance tends to zero. Rather, the information about the presence or absence of inhomogeneities must be contained entirely in the constitutive equations. The basic starting point for Noll's theory is the concept of *material isomorphism*. To make matters more specific, consider the case of a purely elastic material with constitutive law given by

$$\mathbf{t} = \mathbf{t}(\mathbf{F}, \mathbf{X}). \quad (2.1)$$

Here \mathbf{t} represents the Cauchy stress, and \mathbf{F} is the deformation gradient evaluated at the body point \mathbf{X} . We ask the question: given two body points, \mathbf{X}_1 and \mathbf{X}_2 , are they made of the same material? One might think that this question has an easy answer, namely: assume the constitutive law to be written for some reference configuration in cartesian coordinates, and that the two functions $\mathbf{t}_1(\mathbf{F}) = \mathbf{t}(\mathbf{F}, \mathbf{X}_1)$ and $\mathbf{t}_2(\mathbf{F}) = \mathbf{t}(\mathbf{F}, \mathbf{X}_2)$ are identical to each other. We might then conclude that the two points are made of the same material. We immediately see, however, that this trial definition reveals its own weakness: changing the reference configuration, the functions will no longer be identical. Nevertheless, the following will be true: if for *some* reference configuration these functions are identical, then there must exist in the body a linear map \mathbf{P}_{12} between the tangent spaces (“infinitesimal neighborhoods”) of \mathbf{X}_1 and \mathbf{X}_2 , such that

$$\mathbf{t}(\mathbf{F}\mathbf{P}_{12}) = \mathbf{t}(\mathbf{F}, \mathbf{X}_2) \quad \text{for all } \mathbf{F}. \quad (2.2)$$

The physical meaning of \mathbf{P}_{12} is the following: the material at point \mathbf{X}_1 is the same as at \mathbf{X}_2 if, and only if, a small neighborhood of \mathbf{X}_1 can be grafted perfectly around \mathbf{X}_2 , after having been deformed to the extent \mathbf{P}_{12} , so that the behavior around \mathbf{X}_2 remains unchanged. The responses of \mathbf{X}_1 and \mathbf{X}_2 are thus identical, modulo a constant preimposed deformation. The map \mathbf{P}_{12} is called a *material isomorphism*. A body is said to be *materially uniform* if all its points are pairwise materially isomorphic.

If the material isomorphisms $\mathbf{P}_{\mathbf{X}\mathbf{Y}}$ can be chosen so as to depend smoothly on \mathbf{X} and \mathbf{Y} , the body is said to be smoothly materially uniform, a property often implicitly assumed.

A central point of the geometric theory results from the fact that the material isomorphisms are, in general, not unique. Indeed, if we identify \mathbf{X}_2 with \mathbf{X}_1 in Eq. (2.2), we conclude that every material symmetry is a material automorphism, and vice versa. Now, let \mathbf{G}_1 and \mathbf{G}_2 denote elements of the material symmetry groups \mathcal{G}_1 and \mathcal{G}_2 , at \mathbf{X}_1 and \mathbf{X}_2 , respectively. Then, given a material isomorphism \mathbf{P}_{12} , the map

$$\mathbf{P}'_{12} = \mathbf{G}_2\mathbf{P}_{12}\mathbf{G}_1 \quad (2.3)$$

is also a material isomorphism. The collection \mathcal{P}_{12} of all material isomorphisms is, therefore,

$$\mathcal{P}_{12} = \mathcal{G}_2\mathbf{P}_{12} = \mathbf{P}_{12}\mathcal{G}_1 = \mathcal{G}_2\mathbf{P}_{12}\mathcal{G}_1, \quad (2.4)$$

and the groups themselves are conjugate by any isomorphism:

$$\mathcal{G}_2 = \mathbf{P}_{12}\mathcal{G}_1\mathbf{P}_{12}^{-1}. \quad (2.5)$$

Having thus settled the question of uniformity (“same material at all body points”), we may ask: does there exist a reference configuration for which material isomorphisms between all pairs of points exist that look simultaneously like the identity? If the answer to this question is “yes”, then the body is said to be *homogeneous*, and any configuration with the above property is called a homogeneous configuration. We clearly see here the kinship of this notion with that of a defective lattice: if half a row of atoms is missing in an otherwise regular lattice, no deformation can possibly restore the regular arrangement. We can pictorially say that in a homogeneous configuration (if it exists) the uniform body structure has been straightened. It may be possible, on the contrary, to straighten the body structure by chunks only, in which case the uniform body is said to be *locally homogeneous* (Noll, 1967). A good example of this situation is the metal ring already mentioned. Without actually cutting it, it is impossible to render it straight. But any arbitrary sector of the ring can be straightened at once.

The body manifold \mathcal{B} equipped with the collection of all possible material isomorphisms is an example of a geometrical object known as a *groupoid*, whose structure group is the typical symmetry group of the material. A concrete way to obtain a grasp of this structure consists of adopting once and for all a fixed body point, \mathbf{X}_0 , as reference. Choosing now a basis \mathbf{e}_0 for the tangent space at \mathbf{X}_0 , the collection $\mathcal{P}_{0,\mathbf{X}}$ of all material isomorphisms between \mathbf{X}_0 and a variable point $\mathbf{X} \in \mathcal{B}$ determines a collection $\mathcal{F}_G(\mathcal{B})$ of bases at \mathbf{X} , materially compatible with \mathbf{e}_0 . This collection is a subset of the frame bundle $\mathcal{F}(\mathcal{B})$, which consists of *all*

possible bases at all points. Technically, the object obtained by reducing the frame bundle to a more restricted bundle controlled by a subgroup \mathcal{G} of the general linear group is called a \mathcal{G} -structure. The notion of local homogeneity discussed above turns out to be equivalent to the integrability of this \mathcal{G} -structure.

To visualize a more definite measure of possible inhomogeneity, consider the case of a triclinic solid, that is, a material with no non-trivial symmetries. In this case, one may proceed as follows: As before, a body point \mathbf{X}_0 is chosen once and for all as reference. Since the material isomorphisms are now unique (the symmetry group being trivial), the unique field of material isomorphisms determines a unique smooth distant parallelism on the body. We call it *material parallelism*, since it is ultimately dictated by the constitutive equation alone. The realization of this parallelism is the following: a vector \mathbf{v}_X at \mathbf{X} is materially parallel to a vector \mathbf{v}_Y at \mathbf{Y} if

$$\mathbf{v}_Y = \mathbf{P}_{XY} \mathbf{v}_X. \quad (2.6)$$

Intuitively, due to the “transplant” or “graft” operation \mathbf{P}_{XY} , the vector \mathbf{v}_X is transformed into the vector \mathbf{v}_Y . This parallelism uniquely determines a *material connection*, with Christoffel symbols given by

$$\Gamma_{IK}^J = -(P^{-1})_I^z \frac{\partial P_z^J}{\partial X_K}, \quad (2.7)$$

where Greek indices represent components at \mathbf{X}_0 and Latin indices are components at \mathbf{X} in some coordinate systems (X^α) and (X^I) , respectively.

In this case, the integrability condition (and, hence local homogeneity) reduces to the vanishing of the torsion tensor

$$\tau_{IK}^J = \Gamma_{IK}^J - \Gamma_{KI}^J \quad (2.8)$$

of the material connection. In terms of the field of bases introduced above, this condition means that this field is holonomic, namely, it is a natural basis of some local coordinate system.

3. Unisymmetric and homosymmetric bodies

In Section 2, the notion of the homogeneity was presented as a property that uniform bodies may or may not possess. Accordingly, it would appear that FGMs, which are essentially non-uniform by construction, cannot be subjected to a similar treatment. On the contrary, the presence of residual stresses, which in the case of uniform materials manifests itself as an inhomogeneity, is of paramount importance in FGMs. In this section, therefore, we attempt to extend the notion of homogeneity to encompass a larger class of materials. To underline the difference between the two situations, we call this property *homosymmetry*.

Definition 3.1. A material body is said to be *unisymmetric* if the material symmetry groups of its points in one (and, therefore, in every) configuration are pairwise conjugate.

Remark 3.2. The conjugation is understood to take place within the general linear group $GL(3)$.

Example 3.3. A solid body with varying material properties, but fully isotropic at each point, is unisymmetric.

Let a unisymmetric body \mathcal{B} be placed in a fixed reference configuration $\kappa_0(\mathcal{B})$. If we select an arbitrary pair of points $\mathbf{X}_1, \mathbf{X}_2$ of \mathcal{B} , with symmetry groups in $\kappa_0(\mathcal{B})$ denoted, respectively, by $\mathcal{G}_1, \mathcal{G}_2$, then, by Definition 3.1, there exists a linear map \mathbf{A} between their tangent spaces

$$\mathbf{A} : T_{\mathbf{X}_1}(\kappa_0(\mathcal{B})) \rightarrow T_{\mathbf{X}_2}(\kappa_0(\mathcal{B})) \tag{3.1}$$

such that

$$\mathcal{G}_2 = \mathbf{A}\mathcal{G}_1\mathbf{A}^{-1}. \tag{3.2}$$

We will call such a map a *symmetry isomorphism*. If \mathbf{X}_2 coincides with \mathbf{X}_1 , we will speak of a *symmetry automorphism*. With some abuse of terminology, we will use these terms to refer both to the map between the tangent spaces and to the group isomorphism they induce.

Remark 3.4. *Physically, a symmetry isomorphism represents how a small neighborhood of \mathbf{X}_1 is to be deformed so that its symmetry group coincides with that of \mathbf{X}_2 .*

If we identify for a moment \mathbf{X}_2 with \mathbf{X}_1 , it is clear that, in addition to those induced by the elements of \mathcal{G}_1 , there are many other symmetry automorphisms. Indeed, any element of the general linear group which commutes with \mathcal{G}_1 will do as a symmetry automorphism. This situation should be contrasted with the conventional notion of *material automorphism* (Noll, 1967), which necessarily coincides with a material symmetry. This greater latitude in the choice of symmetry automorphisms naturally carries over to the choice of symmetry isomorphisms between two different points. Using the result and the terminology of Lemma A.1 (see Appendix A), we conclude:

Lemma 3.5. *Given a symmetry isomorphism \mathbf{A} between two points, \mathbf{X}_i and \mathbf{X}_j , the set \mathcal{A}_{ij} of all possible symmetry isomorphisms is given by*

$$\mathcal{A}_{ij} = \mathbf{A}\mathcal{N}_i = \mathcal{N}_j\mathbf{A} = \mathcal{N}_j\mathbf{A}\mathcal{N}_i, \tag{3.3}$$

where \mathcal{N}_i and \mathcal{N}_j are respectively, the normalizers in $GL(3)$ of \mathcal{G}_i and \mathcal{G}_j (see Appendix A for a definition of the normalizer).

The set \mathcal{A}_{ij} will be referred to as the *conjugator* between \mathcal{G}_i and \mathcal{G}_j .

Remark 3.6. *The normalizer includes automatically all homogeneous dilatations. Although one might be tempted to eliminate once and for all “undesirable” deformations (as far as material symmetries are concerned), we realize that, in the absence of any extra information beyond unisymmetry, this elimination would not be justified, or even possible (but see Remark 5.1).*

Example 3.7. For the triclinic (trivial) symmetry group, the conjugator between any two points is the whole general linear group.

We have so far obtained the following structure, \mathcal{A} , on the material body, induced by its unisymmetry: to every pair of points, $(\mathbf{X}_i, \mathbf{X}_j)$, there corresponds a subset \mathcal{A}_{ij} of $GL(3)$ with the following properties:

1. *Transitivity*

$$\mathcal{A}_{ik} = \mathcal{A}_{ij}\mathcal{A}_{jk} \tag{3.4}$$

for any 3 points $\mathbf{X}_i, \mathbf{X}_j, \mathbf{X}_k$;

2. *Inversivity*

$$\mathcal{A}_{ij} = \mathcal{A}_{ji}^{-1} \tag{3.5}$$

for any 2 points $\mathbf{X}_i, \mathbf{X}_j$;

3. Group property

\mathcal{A}_i is a subgroup, \mathcal{N}_i , of $GL(3)$.

This geometric structure is called a *groupoid* (Mackenzie, 1987). If the dependence of \mathcal{A}_{ij} on \mathbf{X}_i and \mathbf{X}_j is smooth, the structure obtained is a *Lie groupoid*. One way to pin down a groupoid, so as to render it more tractable, consists of choosing at one point, say \mathbf{X}_0 , any particular frame f_0 and use the conjugators to define all possible admissible frames at \mathbf{X}_i by

$$\bar{\mathcal{F}}_i = \mathcal{A}_{0i}f_0. \quad (3.6)$$

In this manner, one obtains a reduction of the principal bundle of frames of $\kappa_0(\mathcal{B})$. This reduction, consisting of all admissible frames attached at each point of the body, is itself a principal bundle or, more specifically, a *G-structure* (Bernard, 1960; Chern, 1966), whose structural group is the normalizer \mathcal{N}_0 .

Remark 3.8. Note that, whereas the groupoid \mathcal{A} depends only on the reference configuration adopted, the associated *G-structure* depends also on the choice of the frame of departure at \mathbf{X}_0 . Different choices, however, lead to equivalent *G-structures* insofar as integrability matters are concerned.

Definition 3.9. A unisymmetric material body is said to be (locally) *homosymmetric* if one (and therefore every one) of its associated *G-structures* is integrable.

Integrability can be understood in the following way: Let a smooth choice of an admissible frame be made at each point of an open neighborhood U in $\kappa_0(\mathcal{B})$. In geometric terms, this is simply a *local section* of the *G-structure*. Obviously, having thus singled out a frame at each point, we have defined a *distant parallelism* on U with Christoffel symbols Γ , which are in general, non-symmetric. In fact, the skew-symmetric part of Γ is a third-order tensor τ known as the *Cartan torsion* of the parallelism. If the torsion vanishes, the parallelism is said to be integrable on U , which in turn means that there exists a smooth change of reference configuration rendering it the ordinary Cartesian parallelism of E^3 . If this can be done for some local section of every open set of a covering of $\kappa_0(\mathcal{B})$, the *G-structure* is integrable. Physically, this means that there exist special reference configurations (henceforth called *homosymmetric configurations*) in which entire chunks of the body (or, possibly, the whole body) have identical (not just conjugate) symmetry groups.

Remark 3.10. Ascertaining the integrability of a *G-structure* is not an easy task, since the choice of local section has considerable freedom within the structural group at each point. Only when the structural group is discrete, the choice is unique. This fortunate situation, however, never arises in unisymmetry considerations, since the normalizer cannot be discrete.

Example 3.11. A triclinic body is automatically homosymmetric because its structural group is the whole of $GL(3)$, so that in any configuration, a trivial global section is available.

4. Unisymmetric homogeneity of elastic solids

If the only information available concerning the mechanical response of a body is its unisymmetry, then nothing more can be said beyond the treatment of the previous section. If, however, the body points are known to exhibit preferred states, then a much sharper characterization can be devised. For specificity, we consider here the case of *elastic solidity*, whereby each point has a *natural or relaxed state* defined uniquely

to within an arbitrary rotation.¹ Moreover, the material symmetry group of a natural state is a subgroup of the orthogonal group.

By virtue of its solidity, and regardless of uniformity or even unisymmetry, a reference configuration of an elastic body is endowed with a unique *Riemannian metric* compatible with its natural states. Indeed, the dot product of two tangent vectors at a point is, by definition, the ordinary cartesian dot product of their “relaxed” images in the natural state. The rotational degree of freedom leaves this result unaffected. Let the *curvature* of this Riemannian metric vanish identically. That would mean that the body can (chunkwise, at least) be brought to a reference configuration at which each point is in a natural state. Such configurations will be called *relaxed or natural configurations*.

Definition 4.1. An elastic solid body is called (locally) *relaxable* if its intrinsic Riemannian metric has vanishing curvature.

Remark 4.2. *Relaxability would correspond, in the context of uniform materials, to the notions of curvilinear or contorted aeolotropy, whereby the stresses can be relieved, but a rotation is still needed to effect the material isomorphism between points. Here, this concept emerges without any further material assumption, beyond that of solidity.*

Let us now assume that the solid body is also unisymmetric. Several combinations of the two independent geometric structures (the *G*-structure of unisymmetry and the Riemannian metric of solidity) can occur, the most stringent of which is contained in the following:

Definition 4.3. An elastic solid body is (locally) *unisymmetrically homogeneous* if it is relaxable and homogeneous, and if the natural configurations of the neighborhoods are also homosymmetric configurations.

In other words, unisymmetrical homogeneity corresponds to the mutual compatibility of the two geometric structures.

Example 4.4. A relaxable triclinic body is automatically unisymmetrically homogeneous. This example is an extreme case in which the difference between ordinary homogeneity and unisymmetrical homogeneity is very obvious and as wide as possible.

Lemma 4.5. *A relaxable isotropic body is automatically unisymmetrically homogeneous.*

Proof. In a relaxed configuration of a neighborhood, all the symmetry groups coincide with the orthogonal group, so that the symmetry isomorphisms can be chosen as the identity. \square

This lemma shows that, for fully isotropic elastic solids, homogeneity (whether of the old or the new vintage) is synonymous with relaxability. In general, in cases such as transverse isotropy and orthotropy, relaxability and unisymmetrical homogeneity are not the same.

Example 4.6. It is easy to imagine a non-uniform elastic solid body made of transversely isotropic points which is at a globally relaxed configuration, but one in which the main axes of transverse isotropy are not parallel. Such a body can then legitimately be said to contain distributed dislocations.

¹ Strictly speaking, elasticity and solidity do not by themselves imply the existence of a natural state (Truesdell and Noll, 1965).

We now address the question as to whether and how the simultaneous compatible integrability of the two geometric structures can be assessed by the integrability of just one structure to be defined. For each $\mathbf{X}_i \in \kappa_0(\mathcal{B})$, let

$$K_i : T_{\mathbf{X}_i}(\kappa_0(\mathcal{B})) \rightarrow \mathbb{R}^3 \tag{4.1}$$

denote a map bringing \mathbf{X}_i to a natural state. As already mentioned, such maps are uniquely defined up to an arbitrary rotation. Given two points \mathbf{X}_i and \mathbf{X}_j with conjugator \mathcal{A}_{ij} , the conjugator $\bar{\mathcal{A}}_{ij}$ between the corresponding natural states is given by

$$\bar{\mathcal{A}}_{ij} = K_j \mathcal{A}_{ij} K_i^{-1}, \tag{4.2}$$

as clarified in the following commutative diagram

$$\begin{array}{ccc} T_{\mathbf{X}_i}(\kappa_0(\mathcal{B})) & \xrightarrow{\mathbf{A} \in \mathcal{A}_{ij}} & T_{\mathbf{X}_j}(\kappa_0(\mathcal{B})) \\ K_i \downarrow & & \downarrow K_j \\ \mathbb{R}^3 & \xrightarrow{\bar{\mathbf{A}} \in \bar{\mathcal{A}}_{ij}} & \mathbb{R}^3 \end{array}$$

Each element $\bar{\mathbf{A}}$ of $\bar{\mathcal{A}}_{ij}$ conjugates two subgroups, $\bar{\mathcal{G}}_i$ and $\bar{\mathcal{G}}_j$, of the orthogonal group. According to Lemma A.2, therefore, to each $\bar{\mathbf{A}}$ there corresponds a unique orthogonal $\bar{\mathbf{Q}}$ which produces the same conjugations $\bar{\mathbf{A}}$. This fact can be obviously used to define an equivalence relation in $\bar{\mathcal{A}}_{ij}$, whereby two elements are equivalent if they have the same orthogonal component in the polar decomposition. We denote by $\bar{\mathcal{A}}'_{ij}$ the corresponding quotient space. Recalling that $\bar{\mathcal{A}}_{ij}$ is given by $\bar{\mathcal{A}}\mathcal{N}(\bar{\mathcal{G}}_i)$, we conclude that $\bar{\mathcal{A}}'_{ij}$ is equivalent to $\bar{\mathbf{Q}}\mathcal{N}'(\bar{\mathcal{G}}_i)$, where $\mathcal{N}'(\bar{\mathcal{G}}_i)$ is the normalizer of $\bar{\mathcal{G}}_i$ within the orthogonal group. Pulling back this construction to $\kappa_0(\mathcal{B})$, we obtain the reduced conjugator

$$\mathcal{A}'_{ij} = K_j^{-1} \bar{\mathcal{A}}'_{ij} K_i, \tag{4.3}$$

which gives rise to a new, reduced, groupoid with structural group $\mathcal{N}'(\bar{\mathcal{G}}_i)$. It is the integrability of this object (or any of its associated G -structures) which represents the notion of unisymmetric homogeneity, as shown in the following proposition:

Proposition 4.7. *A unisymmetric elastic solid body is unisymmetrically homogeneous if, and only if, its associated reduced groupoid \mathcal{A}' is integrable.*

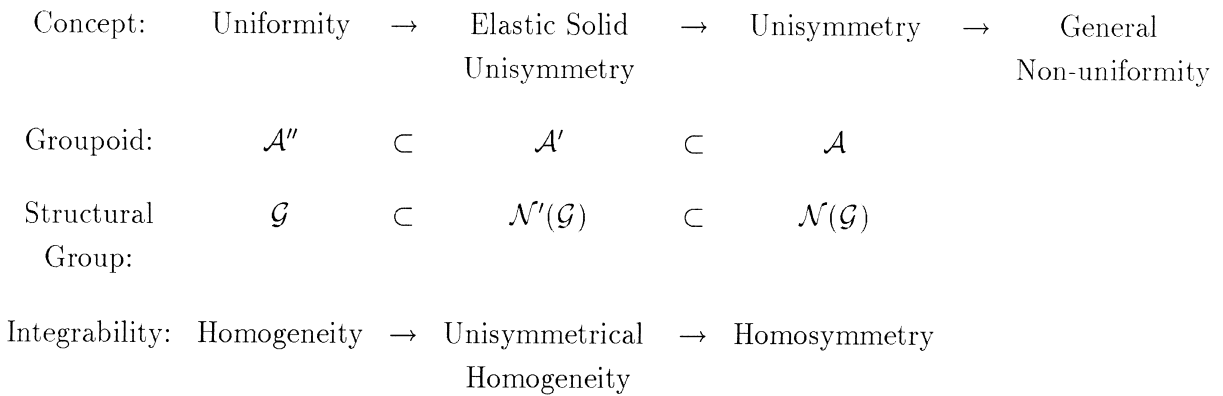
Proof. Since $\mathcal{A}' \subset \mathcal{A}$, the integrability of \mathcal{A}' implies that of \mathcal{A} and, by Definition 3.9, the existence of a homosymmetric configuration, χ_0 say, for a neighborhood U , of each point. Singling out a point $\mathbf{X}_0 \in \chi_0(U)$, let K_0 denote a map bringing it to a natural state. We now change the configuration $\chi_0(\mathcal{B})$ by a homogeneous (i.e., constant gradient) deformation with gradient equal to K_0 . This change of configuration does not alter the (identity) parallelisms. The groupoid \mathcal{A}' conjugates, of course, to a new groupoid which still satisfies Eqs. (4.2) and (4.3). It follows that all points in U must be in the natural state. Conversely, let the body be unisymmetrically homogeneous. There exists then a configuration for which all the maps K_i are orthogonal and, simultaneously, all the unisymmetrical isomorphisms (parallelisms) are trivial. This implies

that the natural state of two points, \mathbf{X}_i and \mathbf{X}_j , in this configuration can be related by the orthogonal tensor $\mathbf{Q}_{ij} = K_j \mathbf{I} K_i^{-1} = K_j K_i^T$. The reduced groupoid in this (and so in every) configuration is obviously integrable by construction. \square

Remark 4.8. *Unlike the normalizer \mathcal{N} of the general case, the normalizer \mathcal{N}' may be discrete, so that, in the case of elastic solids, there will be instances for which the assessment of the integrability, or lack thereof, will turn out to be straightforward.*

5. Further considerations and examples

We have obtained a gradation of geometric structures for an elastic solid which we summarize as follows:



The analysis of a general non-uniform body has not been attempted (for an early attempt in geometric characterization of non-uniformity see Elzanowski and Epstein, 1985). Nevertheless, if the body enjoys the rather weak property of unisymmetry (same “type” of material at all points), then a geometric object already exists for its description: the groupoid \mathcal{A} with structure group $\mathcal{N}(\mathcal{G})$, the normalizer of the typical symmetry group. This is a rather large structural group, allowing for a considerable freedom in the choice of admissible frames. The integrability of this object, guaranteeing the existence of configurations whereby the groups become identical at all points of a neighborhood, would allow for the comparison of points by a wide class of deformation, including dilatations. For special materials, such as elastic solids, some of these deformations may be deemed “undesirable”, since they would imply the coexistence of points in natural and stressed states even in the privileged configurations, guaranteed by the integrability condition. For elastic solids, therefore, a subgroupoid \mathcal{A}' can be constructed with structural group $\mathcal{N}'(\mathcal{G})$, the normalizer of \mathcal{G} within the orthogonal group. The integrability of this new object eliminates the unwanted situations, since it ensures the existence of fully relaxed configurations in which the groups coincide at all points. The non-integrability of \mathcal{A}' can thus be seen as an indication of the existence of distributed dislocations (or other defects possibly causing residual stresses) *in a non-uniform body*. Finally, if the body happens to be uniform, the classical notion of homogeneity is recovered as the integrability of the smaller groupoid \mathcal{A}'' with structural group \mathcal{G} . As far as this smaller structure is concerned, some of the previous isomorphisms permitted by \mathcal{A}' may be expected to be inadmissible. This situation will arise if there exist orthogonal automorphisms of a natural state which do not belong to the symmetry group. In other words, the criterion

of two points having just the same symmetry group may not be as fine as the criterion of having the same constitutive equation. It is quite remarkable, though, that for many types of solids this is not the case, and both criteria give rise to the *same* measure of inhomogeneity. To clarify these matters, a few examples will be studied.

Remark 5.1. *If, for some physical reason, it were possible to choose for each material point a preferential density, then another (larger) groupoid could be constructed, whose structural group is the unimodular part of the normalizer. Its integrability would measure the possibility of achieving a configuration in which each point is at its preferential density while the symmetry groups are identical within a neighborhood. The mathematical possibility also exists of defining an intermediate groupoid based upon the centralizer, rather than the normalizer, of the symmetry group. Its physical significance, as well as that of its integrability, are open to interpretation.*

Remark 5.2. *Given a hyperelastic constitutive equation $W = W(\mathbf{F}, \mathbf{X})$, where W is the stored energy density and \mathbf{F} is the deformation gradient at the point \mathbf{X} , the mere requirement of smoothness of W with respect to \mathbf{X} already has implications as to the conjugability of the symmetry groups at different points. It is to be expected that the symmetry groups must turn out to conjugate almost everywhere. This difficult analytical question deserves further study.*

In the remainder of this section, we consider examples of homogeneity and unisymmetric homogeneity of some classes of elastic solids. From the results listed in the Appendix A, it follows that for the fully *isotropic* class the normalizer \mathcal{N}^t within the orthogonal group coincides with the whole group. From the physical point of view, this means that there is no difference between ordinary (i.e., uniform) homogeneity and unisymmetrical homogeneity. In other words, were we to have established that a body is unisymmetrically homogeneous on the basis of the conjugability of the symmetry groups and the natural states of its points, the awareness that the body is actually uniform would not add any extra information as far as the presence of continuous distributions of inhomogeneities is concerned.

The same result is true for the only other continuous symmetry group of an elastic solid, corresponding to *transverse isotropy*: the group of rotations about a fixed axis. As shown in Appendix A, the orthogonal normalizer in this case, coincides with the group itself, and so there are no extra degrees of freedom left as compared with the case of ordinary (uniform) homogeneity. It is quite remarkable that in these two special cases (full and transverse isotropy), as far as an elastic solid body is concerned, there is no need for the body to be made of the same material at all points in order to define and determine the presence of continuous distributions of inhomogeneities.

We next consider a variety of classes, all of which we have encompassed under the designation of *n-gonal systems*. They consist of material points whose symmetry group in a natural state consists of the rotations generated by successive applications of a rotation of magnitude $2\pi/n$ (for some integer $n > 1$) about a fixed axis. We have shown in Appendix A that the orthogonal normalizer of these groups is the same as that for transverse isotropy, namely, the group of all rotations about the axis. The physical consequence of the fact that the orthogonal normalizer is larger than the symmetry group is the following: If, having determined that the body is unisymmetrically homogeneous, we become aware that it is also uniform, then the possibility exists that, although the main axes of rotation are all parallel in the relaxed configuration, a further adjustment is needed to render the symmetry isomorphisms material isomorphisms. This adjustment may only consist of rotations about the main axis at each point and, therefore, will be generally impossible without stress.

To consider the case of *orthotropic materials*, we discuss now the rhombic system, whose symmetry group consists of just four elements (or eight, if we count those with negative determinant), as detailed in Appendix A. In this case, the orthogonal normalizer coincides with the group itself. Here we have,

therefore, an instance in which the structural group turns out to be discrete and, as a consequence, there is no difference between ordinary (uniform) homogeneity and unisymmetrical homogeneity in this important category of materials. Moreover, the condition of integrability reduces to the vanishing of the torsion of the *unique distant parallelism* available.

Finally, as already pointed out, the *triclinic system* exhibits an orthogonal normalizer which is as large as possible, namely, the whole orthogonal group. Physically, this means that unisymmetrical homogeneity can only detect relaxability, whereby the different points of a neighborhood can be simultaneously brought to a natural state, but an arbitrary rotation will, in general, be needed to bring them into material isomorphism. As in the case of n -agonal symmetry, this extra rotation will in general be impossible without stress (for a two-dimensional setting, see Epstein, 1987). Thus, there is an essential difference between the two kinds of homogeneity in triclinic materials.

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Appendix A

Given a group \mathcal{H} , a fixed element $\mathbf{H} \in \mathcal{H}$, and a subset $\mathcal{G}_0 \subset \mathcal{H}$, the subset

$$\mathcal{G}_1 = \mathbf{H}\mathcal{G}_0\mathbf{H}^{-1} = \{G \in \mathcal{H} \mid G = \mathbf{H}G_0\mathbf{H}^{-1} \text{ for some } G_0 \in \mathcal{G}_0\} \quad (\text{A.1})$$

is called the *conjugate* of \mathcal{G}_0 by \mathbf{H} . The conjugate of a subgroup is again a subgroup.

Two conjugate subgroups are isomorphic, since a conjugation is always bijective (one-to-one and onto) and preserves the group multiplication and the taking of inverses. If $\mathcal{G}_1 = \mathcal{G}_0$, the isomorphism is called an *automorphism*. Conjugation of a subgroup by any one of its own elements is always an automorphism called an *inner automorphism*.

The *normalizer* $\mathcal{N}(\mathcal{G})$ of a subgroup $\mathcal{G} \subset \mathcal{H}$ consists of all the elements of \mathcal{H} which, by conjugation, produce automorphisms of \mathcal{G} :

$$\mathcal{N}(\mathcal{G}) = \{\mathbf{H} \in \mathcal{H} \mid \mathbf{H}\mathbf{G}\mathbf{H}^{-1} \in \mathcal{G} \text{ for all } G \in \mathcal{G}\}. \quad (\text{A.2})$$

This condition can be briefly written as:

$$\mathbf{H}\mathcal{G} = \mathcal{G}\mathbf{H}, \quad (\text{A.3})$$

so we may say that the elements of the normalizer commute with the subgroup. This should not be confused with those elements of \mathcal{H} which commute with every element of \mathcal{G} . They constitute the *centralizer* $\mathcal{C}(\mathcal{G})$ of \mathcal{G} in \mathcal{H} :

$$\mathcal{C}(\mathcal{G}) = \{\mathbf{H} \in \mathcal{H} \mid \mathbf{H}\mathbf{G}\mathbf{H}^{-1} = \mathbf{G} \text{ for every } G \in \mathcal{G}\}. \quad (\text{A.4})$$

It is not difficult to verify that both $\mathcal{N}(\mathcal{G})$ and $\mathcal{C}(\mathcal{G})$ are themselves subgroups of \mathcal{H} , and that the normalizer includes both the original subgroup and its centralizer, viz:

$$\mathcal{G} \cup \mathcal{C}(\mathcal{G}) \subset \mathcal{N}(\mathcal{G}). \quad (\text{A.5})$$

This union can, and will, also be understood in the sense of *subgroup union*, which consists not just of the elements belonging to either subgroup, but also of all the elements of \mathcal{H} obtained by group multiplication

of any finite number of elements from both subgroups taken in any order. Thus, the union turns out to be a subgroup. In our case, because of the commutative property of the centralizer, only one factor is needed from each group, i.e.,

$$\mathcal{G} \cup \mathcal{C}(\mathcal{G}) = \{\mathbf{H} \in \mathcal{H} \mid \mathbf{H} = \mathbf{G}\mathbf{C} \text{ for some } \mathbf{G} \in \mathcal{G} \text{ and for some } \mathbf{C} \in \mathcal{C}(\mathcal{G})\}. \quad (\text{A.6})$$

Lemma A.1. *Given two conjugate subgroups, \mathcal{G}_0 and \mathcal{G}_1 , of a group \mathcal{H} , and given any particular conjugation $\mathbf{M} \in \mathcal{H}$, the set \mathcal{M} of all possible conjugations between the sub-groups is given by*

$$\mathcal{M} = \mathbf{M}\mathcal{N}(\mathcal{G}_0) = \mathcal{N}(\mathcal{G}_1)\mathbf{M} = \mathcal{N}(\mathcal{G}_1)\mathbf{M}\mathcal{N}(\mathcal{G}_0). \quad (\text{A.7})$$

(The set \mathcal{M} will be called the *conjugator* from \mathcal{G}_0 to \mathcal{G}_1 .)

Proof. By direct verification, using the definition of normalizer. \square

We may say, then, that the degrees of freedom afforded to a conjugator from a subgroup to any other, are measured at least by the subgroup itself and its centralizer. In general, however, the normalizer is strictly larger than the union of the subgroup with its centralizer.

We are particularly interested in the application of these concepts to the general linear group in three dimensions, $\text{GL}(3)$, represented by all non-singular matrices of order 3. Clearly, the centralizer of any subgroup of $\text{GL}(3)$ contains at least all scalar matrices, that is, scalar multiples of the identity matrix \mathbf{I} . Of particular relevance to our considerations are the subgroups of the orthogonal group $\mathcal{O}(3) \subset \text{GL}(3)$ defined as

$$\mathcal{O}(3) = \{\mathbf{Q} \in \text{GL}(3) \mid \mathbf{Q}^{-1} = \mathbf{Q}^T\}. \quad (\text{A.8})$$

The subgroups of $\mathcal{O}(3)$ enjoy the remarkable property embodied in the following lemma.

Lemma A.2. *Let $\mathcal{G}_1, \mathcal{G}_2 \subset \mathcal{O}(3)$ be orthogonal subgroups. Then, every isomorphism between \mathcal{G}_1 and \mathcal{G}_2 by conjugation with an element $\mathbf{H} \in \text{GL}(3)$ is also an orthogonal isomorphism, namely, a conjugation by some element $\mathbf{R} \in \mathcal{O}(3)$. Moreover, \mathbf{R} is uniquely determined by \mathbf{H} through polar decomposition.*

Proof. This lemma can be proved in at least three different ways: by representation in an eigenbasis of the symmetric polar component, by a clever use of the uniqueness of polar decomposition (as done by Coleman and Noll, 1964; see also Truesdell and Noll, 1965), or, as in what follows, by the use of the Cayley–Hamilton theorem. First, we note that, since the elements of \mathcal{G}_2 are orthogonal matrices, we must have for every $\mathbf{Q} \in \mathcal{G}_1$:

$$(\mathbf{H}\mathbf{Q}\mathbf{H}^{-1})^{-1} = (\mathbf{H}\mathbf{Q}\mathbf{H}^{-1})^T, \quad (\text{A.9})$$

whence

$$(\mathbf{H}^T\mathbf{H})\mathbf{Q}(\mathbf{H}^T\mathbf{H})^{-1} = \mathbf{Q} \quad \text{for all } \mathbf{Q} \in \mathcal{G}_1. \quad (\text{A.10})$$

In other words, the symmetric positive-definite matrix $\mathbf{H}^T\mathbf{H}$ belongs to the centralizer of \mathcal{G}_1 . But by the polar decomposition theorem, there exists a unique orthogonal matrix \mathbf{R} and a unique positive-definite symmetric matrix \mathbf{S} such that $\mathbf{H} = \mathbf{R}\mathbf{S}$. Therefore,

$$\mathbf{S}^2 = \mathbf{S}^T\mathbf{S} = \mathbf{H}^T\mathbf{R}\mathbf{R}^T\mathbf{H} = \mathbf{H}^T\mathbf{H} \in \mathcal{C}(\mathcal{G}_1), \quad (\text{A.11})$$

which means that \mathbf{S}^2 commutes with every element of \mathcal{G}_1 . We need to show that \mathbf{S} itself has the same property. By the theorem of Cayley–Hamilton, \mathbf{S} satisfies the identity:

$$-\mathbf{S}^3 + I_1\mathbf{S}^2 - I_2\mathbf{S} + I_3\mathbf{I} = 0, \quad (\text{A.12})$$

where I_1, I_2, I_3 are the three invariants of \mathbf{S} , all of which are strictly positive. Since $\mathbf{S}^2\mathbf{Q} = \mathbf{Q}\mathbf{S}^2$ for every $\mathbf{Q} \in \mathcal{G}_1$, it follows that

$$\begin{aligned} \mathbf{S}\mathbf{Q}(\mathbf{S}^2 + I_2\mathbf{I}) &= \mathbf{S}^3\mathbf{Q} + I_2\mathbf{S}\mathbf{Q} = (I_1\mathbf{S}^2 + I_3\mathbf{I})\mathbf{Q} \\ &= \mathbf{Q}(I_1\mathbf{S}^2 + I_3\mathbf{I}) = \mathbf{Q}\mathbf{S}^3 + I_2\mathbf{Q}\mathbf{S} = \mathbf{Q}\mathbf{S}(\mathbf{S}^2 + I_2\mathbf{I}). \end{aligned} \tag{A.13}$$

But I_2 being strictly positive, the matrix $\mathbf{S}^2 + I_2\mathbf{I}$ cannot be singular, which implies that $\mathbf{S}\mathbf{Q} = \mathbf{Q}\mathbf{S}$, as was to be proved. Therefore,

$$\mathbf{H}\mathbf{Q}\mathbf{H}^{-1} = \mathbf{R}\mathbf{S}\mathbf{Q}\mathbf{S}^{-1}\mathbf{R}^T = \mathbf{R}\mathbf{Q}\mathbf{S}\mathbf{S}^{-1}\mathbf{R}^T = \mathbf{R}\mathbf{Q}\mathbf{R}^T. \quad \square \tag{A.14}$$

We now explicitly describe the normalizer and centralizer of a few orthogonal subgroups of interest in applications to solids. In all cases, it turns out that the normalizer is exactly equal to the group union of the subgroup itself with its centralizer.

Remark A.3. *It is straightforward matter to show that a necessary and sufficient condition for this to be the case is that every automorphism, be also an inner automorphism, a condition stronger than that used in the previous lemma.*

Example A.4 (The orthogonal group $\mathcal{O}(3)$). *Centralizer*

An element \mathbf{C} of the centralizer of $\mathcal{O}(3)$ must, by definition, commute with every orthogonal matrix \mathbf{Q} . In particular, choosing \mathbf{Q} alternatively as the diagonal matrices

$$\mathbf{Q} = \text{diag}(1, -1, -1), \text{diag}(-1, 1, -1), \text{diag}(-1, -1, 1), \tag{A.15}$$

we deduce that \mathbf{C} must be diagonal. Choosing now

$$\mathbf{Q} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix},$$

it follows that \mathbf{C} must be a scalar matrix. Further restrictions cannot be expected, since the centralizer automatically contains all scalar matrices.

Normalizer

By the same argument as in Lemma A.2, we conclude that if \mathbf{N} is in the normalizer, then $\mathbf{N}^T\mathbf{N}$ is in the centralizer. Therefore, $\mathbf{N}^T\mathbf{N}$ is a positive scalar matrix and so is its square root, \mathbf{S} . By polar decomposition, there exists an orthogonal matrix \mathbf{R} such that $\mathbf{N} = \mathbf{R}\mathbf{S}$. Vice versa, if $\mathbf{N} = \mathbf{R}\mathbf{S}$ for some orthogonal \mathbf{R} and some scalar matrix \mathbf{S} , then \mathbf{N} conjugates $\mathcal{O}(3)$ onto itself, which shows that the normalizer consists exactly of all products of orthogonal and scalar matrices. Finally, since the only scalar orthogonal matrices are \mathbf{I} and $-\mathbf{I}$, the orthogonal part of the normalizer coincides with the orthogonal group.

Example A.5 (The group \mathcal{O}_x of rotations about a fixed axis x). *Centralizer \mathcal{O}_x* can be represented by all matrices of the form:

$$\mathbf{Q} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & \sin \theta \\ 0 & -\sin \theta & \cos \theta \end{pmatrix}, \quad 0 \leq \theta < 2\pi.$$

First, choosing $\mathbf{Q} = \text{diag}(1, -1, -1)$, we obtain that $\mathbf{C} \in \mathcal{C}(\mathcal{O}_x)$ must be of the form

$$\mathbf{C} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & c \\ 0 & d & e \end{pmatrix} \quad a, b, c, d, e \in \mathbb{R}.$$

Now using an arbitrary \mathbf{Q} from the group, it follows that $b = e$, and $c = -d$. No further reduction is possible, so the most general form of an element in the centralizer is

$$\begin{pmatrix} a & 0 & 0 \\ 0 & b & c \\ 0 & -c & b \end{pmatrix}, \quad a, b, c \in \mathbb{R}.$$

Normalizer

Specifically, for each θ there must exist a ϕ such that

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & \sin \theta \\ 0 & -\sin \theta & \cos \theta \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \phi & \sin \phi \\ 0 & -\sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix},$$

where a_{ij} denote the entries in a matrix \mathbf{A} in the normalizer.

By polar decomposition in a two-dimensional subspace, and using the arguments of the previous lemma, we conclude that the lower right submatrix of \mathbf{A} must be the product of a positive scalar matrix times an orthogonal matrix in two dimensions. Note that ϕ cannot be identically zero for all θ . Operating on the remaining submatrices, one obtains that necessarily $a_{12} = a_{13} = a_{21} = a_{31} = 0$. That is, the most general form of matrix \mathbf{A} of the normalizer is

$$\mathbf{A} = \begin{pmatrix} a & 0 & 0 \\ 0 & \lambda \cos \theta & \lambda \sin \theta \\ 0 & -\lambda \sin \theta & \lambda \cos \theta \end{pmatrix}, \quad a, \theta \in \mathbb{R}, \quad \lambda \in \mathbb{R}^+.$$

But this is precisely the form of the general matrix of the centralizer (with the identification $\lambda^2 = b^2 + c^2$). In this case, therefore, the normalizer coincides with the centralizer. The orthogonal part of the normalizer coincides with the original group.

Example A.6 (*The n -agonal groups*). We call n -agonal the group of rotations generated by a rotation of magnitude $2\pi/n$ (with n an integer greater than 1) about a fixed axis x .

Centralizer:

We distinguish the two cases $n = 2$ and $n > 2$. For $n = 2$ we obtain by direct calculation

$$\mathbf{C} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & c \\ 0 & d & e \end{pmatrix}, \quad a, b, c, d, e \in \mathbb{R}.$$

For $n > 2$ we obtain

$$\mathbf{C} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & c \\ 0 & -c & b \end{pmatrix}, \quad a, b, c \in \mathbb{R}.$$

Normalizer:

In all cases, the normalizer is equal to the corresponding centralizer. The orthogonal part of the normalizer is the group of *all* rotations about x .

Example A.7 (*The rhombic group*). The rhombic group can be represented by the four matrices

$$\mathbf{Q}_1 = \mathbf{I}, \quad \mathbf{Q}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{Q}_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{Q}_4 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

This is a discrete Abelian group. A direct computation of all the possibilities reveals that both the centralizer and the normalizer consist of all the diagonal matrices (not necessarily scalar). The orthogonal normalizer coincides with the original group.

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