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3D extension of Tensorial Polar Decomposition. Application to (photo-)elasticity tensors

Extension 3D de la Décomposition Polaire Tensorielle. Application aux tenseurs de (photo-)elasticité

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A B S T R A C T

The orthogonalized harmonic decomposition of symmetric fourth-order tensors (i.e. having major and minor indicial symmetries, such as elasticity tensors) is completed by a representation of harmonic fourth-order tensors $\mathbb{H}$ by means of two second-order harmonic (symmetric deviatoric) tensors only. A similar decomposition is obtained for non-symmetric tensors (i.e. having minor indicial symmetry only, such as photo-elasticity tensors or elasto-plasticity tangent operators) introducing a fourth-order major antisymmetric traceless tensor $\mathbb{Z}$. The tensor $\mathbb{Z}$ is represented by means of one harmonic second-order tensor and one antisymmetric second-order tensor only. Representations of totally symmetric (rari-constant), symmetric and major antisymmetric fourth-order tensors are simple particular cases of the proposed general representation. Closed-form expressions for tensor decomposition are given in the monoclinic case. Practical applications to elasticity and photo-elasticity monoclinic tensors are finally presented.

R É S U M É

La décomposition harmonique orthogonalisée des tenseurs symétriques d'ordre quatre (ayant les symétries majeures et mineures, tels que le tenseur d'élasticité) est complétée par une représentation des tenseurs harmoniques d'ordre quatre $\mathbb{H}$ à l'aide de deux tenseurs harmoniques (symétriques déviatoriques) d'ordre deux. Une décomposition similaire est obtenue pour les tenseurs non symétriques (ayant uniquement la symétrie mineure, tels que ceux rencontrés en photo-élasticité et en élasto-plasticité), introduisant un tenseur antisymétrique majeur à traces nulles $\mathbb{Z}$. Le tenseur $\mathbb{Z}$ est représenté par deux tenseurs d'ordre deux, le premier harmonique et le second antisymétrique. Les représentations des tenseurs d'ordre quatre complètement symétriques (rari-constants), symétriques et antisymétriques majeurs sont des cas particuliers simples de la représentation proposée.

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Les expressions analytiques de la décomposition correspondante dans le cas monoclinique sont obtenues et appliquées à l'élasticité et à la photo-élasticité monocliniques.

1. Introduction

Fourth-order tensors are symmetric in elasticity (the corresponding vector space is denoted $\mathbb{E}\mathrm{la}$ [1,2]); they are possibly non-symmetric in rate form elasto-plasticity or in photo-elasticity (the corresponding vector space is denoted by $\mathbb{G}\mathrm{el}$ [3]). Even if they are commonly used in mechanics of materials, their inner structure still needs to be more precisely described in 3D.

In 3D, the well-known harmonic decomposition [4–8,1,9] is often completed by the Cartan decomposition of its fourth-order harmonic part $\mathbb{H}$ (traceless totally symmetric fourth-order tensor, the corresponding vector space being denoted by $\mathbb{H}\mathrm{rm}$): this decomposition, quite complex,[1] has been useful for the determination of the irreducible symmetry classes of elastic and piezoelectric solids [1,13]. An integrity basis of tensor spaces is given in [14]. It is defined using group representation and polynomial invariants [15–17]. Reference [18] gives a direct application to harmonic fourth-order tensors.

In 2D, alternative descriptions have been introduced [19–22], shown to be related both to the harmonic decomposition [23] and to the Kelvin decomposition of the harmonic tensor [24]. It is nevertheless important to point out that among those descriptions, the so-called polar decomposition of 2D symmetric fourth-order tensors of Verchery implicitly contains the inner structure of 2D harmonic fourth-order tensors. For instance, the corresponding rewriting of 2D harmonic fourth-order tensors $\in \mathbb{H}\mathrm{rm}^{(2D)}$ recently performed in [24] simply reads

$$\mathbb{H} = \mathbf{h}_0 \otimes \mathbf{h}_0 - \frac{1}{2}\mathbf{h}_0 : \mathbf{h}_0\, \mathbb{J}^{2D} \qquad \mathrm{tr}_{12}\,\mathbb{H} = \mathrm{tr}_{13}\,\mathbb{H} = 0 \tag{1}$$

giving the general expression of any 2D harmonic fourth-order tensor as a function of one traceless symmetric (harmonic) second-order tensor $\mathbf{h}_0 = \mathbf{h}_0'$ only. In Eq. (1), the fourth-order tensor $\mathbb{J}^{2D} = \mathbb{I} - \frac{1}{2}\mathbf{1} \otimes \mathbf{1}$ is such that $(.)' = \mathbb{J}^{2D} : (.) = (.) - \frac{1}{2}\,\mathrm{tr}(.)\,\mathbf{1}$ stands for the 2D deviatoric part of second-order tensors.

Combined with standard harmonic decomposition, Eq. (1) of Tensorial Polar Decomposition implies that any 2D symmetric fourth-order tensor can be expressed by means of two scalar invariants (frame independent) and of two symmetric deviatoric (harmonic) second-order tensors only $\mathbf{h}_0, \mathbf{h}_1 \in \mathbf{Dev}^{(2D)}$, with no remaining strictly fourth-order tensorial part – as thanks to Eq. (1), $\mathbb{H} \in \mathbb{H}\mathrm{rm}^{(2D)}$ is expressed by means of the single second-order tensor $\mathbf{h}_0$. Using direct sums, this means that $\mathbb{E}\mathrm{la}^{(2D)} = \mathrm{R} \oplus \mathrm{R} \oplus \mathbf{Dev}^{(2D)} \oplus \mathbf{Dev}^{(2D)}$ (with $\mathbb{H}\mathrm{rm}^{(2D)} = \mathbf{Dev}^{(2D)}$) [24] instead of the standard harmonic decomposition $R \oplus R \oplus \mathbf{Dev}^{(2D)} \oplus \mathbb{H}\mathrm{rm}^{(2D)}$ for 2D symmetric fourth-order tensors, if R denotes the real (scalar) vector space.

The 2D polar decomposition as well as its tensorial rewriting make explicitly appear polar invariants and their link with symmetry classes [21]. This property also stands for non-symmetric tensors, as shown in [25] by means of complex variables changes for the two cases *i*) of fourth-order tensors having major indicial symmetry only and *ii*) of fourth-order tensors having minor indicial symmetry only (case recalled next, Eq. (5)). As the polar decomposition method for non-symmetric tensors had no tensorial writing counterpart, our first action will be to give such a 2D formula (as novel Eq. (6)). The question then will be how to extend to 3D the refined results (Eq. (1)) on the inner structure of 2D harmonic tensors, and more generally how to extend the refined results of Tensorial Polar Decomposition (Eqs. (4) and (6)) to 3D elasticity tensor $\in \mathbb{E}\mathrm{la}$ and to 3D non-symmetric tensors $\in \mathbb{G}\mathrm{el}$.

Those questions have a close link with the description of elasticity symmetry classes [21,18,23] and with the definition of invariants for fourth-order tensors. It is not the purpose here to debate this point in the 3D case. Note nevertheless that in 2D, the definition of polar invariants by Verchery and Vannucci is strongly related to the orthonormalization of the harmonic decomposition performed for 2D tensors [24] (section 2.3). In order to extend polar decomposition to 3D, in a tensorial framework, one proposes therefore:

1. to make appear polar moduli r_n in Backus orthogonalized harmonic decomposition for symmetric tensors $\mathbb{S}$ (having minor and major indicial symmetries, section 4),
2. to express the harmonic tensors $\mathbb{H}$ by means of symmetric deviatoric second-order tensors only (section 5, generalization to 3D of Eq. (1)),
3. to apply the same procedure to (major) antisymmetric tensors $\mathbb{A}$ (having minor indicial symmetry, section 6).

[1] See [10–12] for its link with group representation theory.

2. 2D case: Tensorial Polar Decomposition

In 2D, such as in the case of planar elasticity, a symmetric tensor $\mathbb{S}$ having both minor and major indicial symmetries has six independent components S_{ijkl}. A 2D tensor $\mathbb{T}$ having only minor symmetries has nine independent components T_{ijkl}. Polar formalism defines in a closed form their dependency with respect to the frame angle θ by making appear invariants of two types: polar moduli or angular differences [20]. Scalars t_n, r_n, φ_n are the notations used next for the material parameters of 2D anisotropic elasticity or photo-elasticity (see [25]). The First question is then how to define a tensorial representation that makes directly appear the parameters (and the invariants) of polar decomposition theory both in the symmetric case (problem recently solved [24], Eq. (4)) and in the case with minor indicial symmetry only.

2.1. Symmetric tensors $\mathbb{S}$

Let consider a 2D symmetric fourth-order tensor $\mathbb{S}$ having both minor and major indicial symmetries ($S_{ijkl} = S_{klij} = S_{ijlk} = S_{jikl}$). The basic result of the polar formalism is the expression of the Cartesian components of the 2D symmetric tensor $\mathbb{S}$ in terms of polar parameters, in a frame rotated through an angle θ [20,21]:

$$\begin{aligned}
S_{1111}(\theta) &= t_0 + 2t_1 + r_0 \cos 4(\varphi_0 - \theta) + 4r_1 \cos 2(\varphi_1 - \theta)\\
S_{1112}(\theta) &= r_0 \sin 4(\varphi_0 - \theta) + 2r_1 \sin 2(\varphi_1 - \theta)\\
S_{1122}(\theta) &= -t_0 + 2t_1 - r_0 \cos 4(\varphi_0 - \theta)\\
S_{1212}(\theta) &= t_0 - r_0 \cos 4(\varphi_0 - \theta)\\
S_{1222}(\theta) &= -r_0 \sin 4(\varphi_0 - \theta) + 2r_1 \sin 2(\varphi_1 - \theta)\\
S_{2222}(\theta) &= t_0 + 2t_1 + r_0 \cos 4(\varphi_0 - \theta) - 4r_1 \cos 2(\varphi_1 - \theta)
\end{aligned} \tag{2}$$

t_0 and t_1 contributions are frame independent (they define the isotropic part of $\mathbb{S}$ as a generalization of Lamé constants to anisotropy), the r_1 terms rotates in $\cos 2(\varphi_1 - \theta)$ and $\sin 2(\varphi_1 - \theta)$ as second-order tensors do (see Eq. (3)), the r_0 term rotates twice more in $\cos 4(\varphi_0 - \theta)$ and $\sin 4(\varphi_0 - \theta)$. In a given frame θ, the knowledge of the six independent coefficients of any 2D symmetric tensor $\mathbb{S}$ is equivalent to the knowledge of the five invariants $(t_0, t_1, r_0, r_1, \varphi_0 - \varphi_1)$ and of one angle, either $\varphi_0 - \theta$ or $\varphi_1 - \theta$.

Introducing the two second-order deviatoric tensors (of unit J_2-norm, $n = 0, 1$):

$$\mathbf{R}_n = \mathbf{R}'_n = \begin{pmatrix} \cos 2(\varphi_n - \theta) & \sin 2(\varphi_n - \theta) \\ \sin 2(\varphi_n - \theta) & -\cos 2(\varphi_n - \theta) \end{pmatrix} \qquad \text{with} \quad J_2(\mathbf{R}'_n) = \sqrt{\frac{1}{2}\mathbf{R}'_n : \mathbf{R}'_n} = 1 \tag{3}$$

Eq. (2) can be recast as (see [24])

$$\mathbb{S} = 2t_0 \mathbb{J}^{2D} + 2t_1 \mathbf{1} \otimes \mathbf{1} + 2r_0 \left[\mathbf{R}'_0 \otimes \mathbf{R}'_0 - \mathbb{J}^{2D}\right] + 2r_1 \left(\mathbf{1} \otimes \mathbf{R}'_1 + \mathbf{R}'_1 \otimes \mathbf{1}\right) \tag{4}$$

where the harmonic part (Eq. (1)) has been rewritten as $\mathbb{H} = 2r_0 \left[\mathbf{R}'_0 \otimes \mathbf{R}'_0 - \mathbb{J}^{2D}\right]$ by making polar invariant r_0 appear by setting $\mathbf{h}_0 = \sqrt{2r_0}\,\mathbf{R}'_0$.

2.2. Tensors $\mathbb{T}$ having minor indicial symmetry

Let us now consider a 2D fourth-order tensor $\mathbb{T}$ having only the minor indicial symmetry ($T_{ijkl} = T_{ijlk} = T_{jikl}$), which has then nine independent components, parameterized by frame angle θ. Using the Polar method, such a tensor is obtained in [25] as

$$\begin{aligned}
T_{1111}(\theta) &= t_0 + 2t_1 + r_0 \cos 4(\varphi_0 - \theta) + 2r_1 \cos 2(\varphi_1 - \theta) + 2r_2 \cos 2(\varphi_2 - \theta),\\
T_{1112}(\theta) &= -t_3 + r_0 \sin 4(\varphi_0 - \theta) + 2r_2 \sin 2(\varphi_2 - \theta),\\
T_{1122}(\theta) &= -t_0 + 2t_1 - r_0 \cos 4(\varphi_0 - \theta) + 2r_1 \cos 2(\varphi_1 - \theta) - 2r_2 \cos 2(\varphi_2 - \theta),\\
T_{1211}(\theta) &= t_3 + r_0 \sin 4(\varphi_0 - \theta) + 2r_1 \sin 2(\varphi_1 - \theta),\\
T_{1212}(\theta) &= t_0 - r_0 \cos 4(\varphi_0 - \theta),\\
T_{1222}(\theta) &= -t_3 - r_0 \sin 4(\varphi_0 - \theta) + 2r_1 \sin 2(\varphi_1 - \theta),\\
T_{2211}(\theta) &= -t_0 + 2t_1 - r_0 \cos 4(\varphi_0 - \theta) - 2r_1 \cos 2(\varphi_1 - \theta) + 2r_2 \cos 2(\varphi_2 - \theta),\\
T_{2212}(\theta) &= t_3 - r_0 \sin 4(\varphi_0 - \theta) + 2r_2 \sin 2(\varphi_2 - \theta),\\
T_{2222}(\theta) &= t_0 + 2t_1 + r_0 \cos 4(\varphi_0 - \theta) - 2r_1 \cos 2(\varphi_1 - \theta) - 2r_2 \cos 2(\varphi_2 - \theta)
\end{aligned} \tag{5}$$

where polar moduli r_n are positive invariants. The lack of major indicial symmetry is represented by a non-vanishing term in t_3 and/or by two different terms in (r_1, φ_1) and (r_2, φ_2) in the set of equations (5): major indicial symmetry is recovered when $t_3 = 0$, $r_2 = r_1$ and $\varphi_2 = \varphi_1$.

It can be checked that the intrinsic expression for fourth-order tensors $\mathbb{T}$ having minor indicial symmetry only is

$$\mathbb{T} = 2t_0\,\mathbb{J}^{2D} + 2t_1 \mathbf{1} \otimes \mathbf{1} + t_3 \left[\mathbf{1} \underline{\otimes} \mathbf{A} + \mathbf{A} \underline{\otimes} \mathbf{1}\right] + 2r_0 \left[\mathbf{R}'_0 \otimes \mathbf{R}'_0 - \mathbb{J}^{2D}\right] + 2r_1\, \mathbf{R}'_1 \otimes \mathbf{1} + 2r_2\, \mathbf{1} \otimes \mathbf{R}'_2 \tag{6}$$

with second-order tensors $\mathbf{R}'_0$, $\mathbf{R}'_1$, $\mathbf{R}'_2$ all of the generic form (3). The antisymmetric (frame independent) second-order tensor $\mathbf{A}$ has been introduced, of unit J_2-norm,

$$\mathbf{A} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \qquad \text{with} \quad J_2(\mathbf{A}) = \sqrt{\frac{1}{2}\mathbf{A}:\mathbf{A}} = 1 \tag{7}$$

The proposed (new) 2D decomposition (6) is the intrinsic rewriting of Eq. (5). One will refer to it as Tensorial Polar Decomposition of non-symmetric tensors (i.e. having minor indicial symmetry only). The major symmetry of $\mathbb{T}$ corresponds to $t_3 = 0$, $r_2\mathbf{R}'_2 = r_1\mathbf{R}'_1$. This last tensorial equality is equivalent to $r_2 = r_1$ and $\varphi_2 = \varphi_1$.

2.3. Polar invariants and orthogonality

A feature included in polar decomposition of Verchery and Vannucci is the definition of the so-called polar invariants, of two types: moduli t_n or r_n, and of relative angles $\varphi_n - \varphi_m$. Refer to [25] for the classification of the 2D photo-elasticity material symmetries by means of invariants r_0, r_1, r_2, $\varphi_0 - \varphi_1$, $\varphi_1 - \varphi_2$.

It is worth to point out that the definition of the polar invariants is strongly related to constant norms and to orthogonality – with respect to scalar product :: for fourth-order tensors, $\mathbb{T} :: \mathbb{T} = T_{ijkl}T_{ijkl}$ – of the different tensorial terms introduced in Eq. (6), as each generator $\mathbb{G}^{(n)}$ introduced is orthogonal to all other ones (as detailed in [24] for the symmetric case):

$$\mathbb{J}^{2D} :: \mathbf{1}\otimes\mathbf{1} = \mathbb{J}^{2D} :: \left[\mathbf{1}\underline{\otimes}\mathbf{A} + \mathbf{A}\underline{\otimes}\mathbf{1}\right] = \mathbb{J}^{2D} :: \left[\mathbf{R}'_0\otimes\mathbf{R}'_0 - \mathbb{J}^{2D}\right] = \mathbb{J}^{2D} :: \mathbf{R}'_1\otimes\mathbf{1} = \mathbb{J}^{2D} :: \mathbf{1}\otimes\mathbf{R}'_2 = 0 \tag{8}$$

$$\mathbf{1}\otimes\mathbf{1} :: \left[\mathbf{1}\underline{\otimes}\mathbf{A} + \mathbf{A}\underline{\otimes}\mathbf{1}\right] = \mathbf{1}\otimes\mathbf{1} :: \left[\mathbf{R}'_0\otimes\mathbf{R}'_0 - \mathbb{J}^{2D}\right] = \mathbf{1}\otimes\mathbf{1} :: \mathbf{R}'_1\otimes\mathbf{1} = \mathbf{1}\otimes\mathbf{1} :: \mathbf{1}\otimes\mathbf{R}'_2 = 0 \tag{9}$$

$$\left[\mathbf{1}\underline{\otimes}\mathbf{A} + \mathbf{A}\underline{\otimes}\mathbf{1}\right] :: \left[\mathbf{R}'_0\otimes\mathbf{R}'_0 - \mathbb{J}^{2D}\right] = \left[\mathbf{1}\underline{\otimes}\mathbf{A} + \mathbf{A}\underline{\otimes}\mathbf{1}\right] :: \mathbf{R}'_1\otimes\mathbf{1} = \left[\mathbf{1}\underline{\otimes}\mathbf{A} + \mathbf{A}\underline{\otimes}\mathbf{1}\right] :: \mathbf{1}\otimes\mathbf{R}'_2 = 0 \tag{10}$$

$$\left[\mathbf{R}'_0\otimes\mathbf{R}'_0 - \mathbb{J}^{2D}\right] :: \mathbf{R}'_1\otimes\mathbf{1} = \left[\mathbf{R}'_0\otimes\mathbf{R}'_0 - \mathbb{J}^{2D}\right] :: \mathbf{1}\otimes\mathbf{R}'_2 = \mathbf{R}'_1\otimes\mathbf{1} :: \mathbf{1}\otimes\mathbf{R}'_2 = 0 \tag{11}$$

Note last that using Eq. (3), angular invariants are naturally defined from Tensorial Polar Decomposition as scalar products:

$$\mathbf{R}'_n : \mathbf{R}'_m = 2\cos 2(\varphi_n - \varphi_m) \tag{12}$$

3. Notations for the 3D case

All the fourth-order tensors considered in the present note exhibit minor indicial symmetry. We therefore denote:

- $\mathbb{T}$ as fourth-order tensors having only minor indicial symmetries (non-symmetric fourth-order tensors $\mathbb{T} \in$ vector space $\mathbb{G}$el, using notations of [3]), such as $T_{ijkl} = T_{ijlk} = T_{jikl}$,
- $\mathbb{S}$ as symmetric fourth-order tensors ($\mathbb{S} \in$ vector space $\mathbb{E}$la using notations of [1,18]), such as $S_{ijkl} = S_{klij} = S_{ijlk} = S_{jikl}$,
- $\mathbb{R}$ as rari-constant fourth-order tensors (totally symmetric [26], vector space $\mathbb{R}$ar), having Cauchy indicial symmetries $R_{ijkl} = R_{ikjl}$,
- $\mathbb{H}$ as harmonic fourth-order tensors ($\mathbb{H} \in$ vector space $\mathbb{H}$rm, using notations of [1]), such as $H_{ijkl} = H_{ikjl}$, $H_{kkij} = H_{kikj} = 0$: harmonic tensors are totally symmetric traceless tensors,
- $\mathbb{A}$ as antisymmetric fourth-order tensors, $A_{ijkl} = A_{ijlk} = A_{jikl} = -A_{klij}$,
- $\mathbb{Z}$ as traceless antisymmetric fourth-order tensors, $Z_{ijkl} = Z_{ijlk} = Z_{jikl} = -Z_{klij}$, $Z_{kkij} = Z_{kikj} = 0$.

A 3D non-symmetric tensor $\mathbb{T}$ (having only minor indicial symmetries) has three independent tensorial traces $\mathbf{e} = \mathrm{tr}_{12}\,\mathbb{T}$, $\mathbf{v} = \mathrm{tr}_{13}\,\mathbb{T}$ and $\mathbf{d} = \mathrm{tr}_{34}\,\mathbb{T}$, defining three second-order tensors $\mathbf{e}$, $\mathbf{v}$, $\mathbf{d}$ (of components $e_{ij} = T_{kkij}$, $v_{ij} = T_{kikj}$, $d_{ij} = T_{ijkk}$) with the following names and properties:

- left and right dilatation tensors $\mathbf{e} = \mathbf{e}(\mathbb{T})$ and $\mathbf{d} = \mathbf{d}(\mathbb{T})$ are symmetric second-order tensors for any $\mathbb{T}$, with $\mathbf{e} \neq \mathbf{d}$ when $\mathbb{T}$ is non-symmetric and $\mathbf{e} = \mathbf{d}$ when $\mathbb{T}$ is symmetric,
- Voigt tensor $\mathbf{v} = \mathbf{v}(\mathbb{T})$ is non-symmetric, of antisymmetric part $\mathbf{v}^A$ of components $v^A_{ij} = \frac{1}{2}\left(T_{kikj} - T_{kjki}\right) = \frac{1}{2}\left(A_{kikj} - A_{kjki}\right)$, with therefore $\mathbf{v}$ symmetric when $\mathbb{T}$ is symmetric,
- scalar traces of tensors $\mathbf{e}$ and $\mathbf{d}$ are always equal, $\mathrm{tr}\,\mathbf{e} = \mathrm{tr}\,\mathbf{d} = T_{kkll} = S_{kkll}$; they usually differ from the scalar trace $\mathrm{tr}\,\mathbf{v} = T_{klkl}$ (note that $\mathrm{tr}\,\mathbf{v}^A = 0$).

The tensorial products $\underline{\otimes}$, $\overline{\otimes}$, $\underline{\overline{\otimes}}$ are defined as follows:

$$(\mathbf{X}\underline{\otimes}\mathbf{Y})_{ijkl} = X_{ik}Y_{jl}, \qquad (\mathbf{X}\overline{\otimes}\mathbf{Y})_{ijkl} = X_{il}Y_{jk}, \qquad \mathbf{X}\underline{\overline{\otimes}}\mathbf{Y} = \frac{1}{2}(\mathbf{X}\underline{\otimes}\mathbf{Y} + \mathbf{X}\overline{\otimes}\mathbf{Y}) \tag{13}$$

We also define the special tensorial product $\circledast$ as

$$\mathbf{X}\circledast\mathbf{Y}=\frac{1}{3}\left(\mathbf{X}\otimes\mathbf{Y}+\mathbf{X}\underline{\otimes}\mathbf{Y}+\mathbf{X}\overline{\underline{\otimes}}\mathbf{Y}\right)=\frac{1}{3}\left(\mathbf{X}\otimes\mathbf{Y}+2\,\mathbf{X}\overline{\underline{\otimes}}\mathbf{Y}\right) \tag{14}$$

The totally symmetric (rari-constant) part $\in \mathbb{R}\mathrm{ar}$ of tensor $\mathbf{X}\otimes\mathbf{X}$ is therefore $\mathbf{X}\circledast\mathbf{X}$, so that decomposition of $\mathbf{X}\otimes\mathbf{X}$ into a rari-constant part and an "anti-rari-constant" part is

$$\mathbf{X}\otimes\mathbf{X}=\mathbf{X}\circledast\mathbf{X}+\frac{2}{3}\left(\mathbf{X}\otimes\mathbf{X}-\mathbf{X}\overline{\underline{\otimes}}\mathbf{X}\right) \tag{15}$$

with the fundamental orthogonality property $\mathbf{X}\circledast\mathbf{X}::\left(\mathbf{X}\otimes\mathbf{X}-\mathbf{X}\overline{\underline{\otimes}}\mathbf{X}\right)=0$, using scalar product for fourth-order tensors, $\mathbb{T}::\mathbb{T}=T_{ijkl}T_{ijkl}$.

Remark. $\mathbf{X}\circledast\mathbf{Y}$ is a tensor, it satisfies the change of basis rule ($\forall\mathbf{g}$ orthogonal)

$$\mathbf{g}\star(\mathbf{X}\circledast\mathbf{Y})=(\mathbf{g}\star\mathbf{X})\circledast(\mathbf{g}\star\mathbf{Y})=(\mathbf{g}\cdot\mathbf{X}\cdot\mathbf{g}^{\mathrm{T}})\circledast(\mathbf{g}\cdot\mathbf{Y}\cdot\mathbf{g}^{\mathrm{T}}) \tag{16}$$

in which, for any second-order tensor $(\mathbf{g}\star\mathbf{X})_{ij}=g_{ip}g_{jq}X_{pq}$, and for any fourth-order tensor $(\mathbf{g}\star\mathbb{T})_{ijkl}=g_{ip}g_{jq}g_{kr}g_{ls}T_{pqrs}$. In the rest of the paper, $\mathbf{g}\star$ will denote the action of any rotation[2] $\mathbf{g}$. We will refer to Eq. (16) and to its following particular cases

$$\mathbf{g}\star(\mathbf{1}\circledast\mathbf{X})=\mathbf{1}\circledast(\mathbf{g}\star\mathbf{X})\qquad \mathbf{g}\star(\mathbf{X}\circledast\mathbf{1})=(\mathbf{g}\star\mathbf{X})\circledast\mathbf{1}\qquad \mathbf{g}\star(\mathbf{1}\circledast\mathbf{1})=\mathbf{1}\circledast\mathbf{1} \tag{17}$$

at the end of section 5.

4. Orthogonalized harmonic decomposition of 3D symmetric tensors

Harmonic decomposition of any symmetric fourth-order tensor $\mathbb{S}$ – or of the symmetric part of tensor $\mathbb{T}$ – is its decomposition $R\oplus R\oplus\mathbf{Dev}\oplus\mathbf{Dev}\oplus\mathbb{H}\mathrm{rm}$ in terms of unit second-order tensor $\mathbf{1}$, by means of two scalar invariants $\lambda,\mu\in R$, of harmonic second-order tensors $\boldsymbol{\alpha}',\boldsymbol{\beta}'\in\mathbf{Dev}$ and of a remaining harmonic fourth order harmonic part $\mathbb{H}\in\mathbb{H}\mathrm{rm}$ [4–7]. Using the expression given in [8,1], it is

$$\mathbb{S}=\lambda\mathbf{1}\otimes\mathbf{1}+2\mu\,\mathbf{1}\overline{\underline{\otimes}}\mathbf{1}+\mathbf{1}\otimes\boldsymbol{\alpha}'+\boldsymbol{\alpha}'\otimes\mathbf{1}+\mathbf{1}\underline{\otimes}\boldsymbol{\beta}'+\boldsymbol{\beta}'\underline{\otimes}\mathbf{1}+\mathbf{1}\overline{\otimes}\boldsymbol{\beta}'+\boldsymbol{\beta}'\overline{\otimes}\mathbf{1}+\mathbb{H} \tag{18}$$

harmonic meaning symmetric and traceless, as already mentioned, the harmonic second-order tensors being therefore symmetric and deviatoric. Invariants λ, μ, generalize Lamé constants to anisotropy ($\mathbf{1}\overline{\underline{\otimes}}\mathbf{1}=\mathbb{I}$ is the identity tensor for symmetric fourth-order tensors), the two harmonic second-order tensors $\boldsymbol{\alpha}'$ and $\boldsymbol{\beta}'$ can be derived from the dilatation tensor $\mathbf{d}=\mathbf{d}(\mathbb{S})=\mathrm{tr}_{12}\,\mathbb{S}$ and from the Voigt tensor $\mathbf{v}=\mathbf{v}(\mathbb{S})=\mathrm{tr}_{13}\,\mathbb{S}$ (see [7,18]).

According to Backus [5] and using the special tensorial product $\circledast$ (defined by Eq. (14)), one has for Lamé's λ and μ terms the equality

$$\lambda\mathbf{1}\otimes\mathbf{1}+2\mu\,\mathbf{1}\overline{\underline{\otimes}}\mathbf{1}=r_{\mathrm{c}}\mathbf{1}\circledast\mathbf{1}+2\bar{r}_{\mathrm{c}}\left(\mathbf{1}\otimes\mathbf{1}-\mathbf{1}\overline{\underline{\otimes}}\mathbf{1}\right) \tag{19}$$

if one sets

$$r_{\mathrm{c}}=\lambda+2\mu=\frac{1}{15}\,(\mathrm{tr}\,\mathbf{d}+2\,\mathrm{tr}\,\mathbf{v})\qquad \bar{r}_{\mathrm{c}}=\frac{\lambda-\mu}{3}=\frac{1}{18}\,(\mathrm{tr}\,\mathbf{d}-\mathrm{tr}\,\mathbf{v}) \tag{20}$$

This defines invariants r_{c} and $\bar{r}_{\mathrm{c}}$ – equivalent to the couple λ, μ – for constant terms, the subscript c standing for *constant*, meaning here frame independent. The chosen first letters r and $\bar{r}$ – used instead of the letter t for the 2D constant moduli t_n of section 2 – highlight the fact that $r_{\mathrm{c}}\mathbf{1}\circledast\mathbf{1}$ is rari-constant (totally symmetric) and $2\bar{r}_{\mathrm{c}}\left(\mathbf{1}\otimes\mathbf{1}-\mathbf{1}\overline{\underline{\otimes}}\mathbf{1}\right)$ is anti-rari-constant (it is denoted as asymmetric in reference [5]). The orthogonality property $\mathbf{1}\circledast\mathbf{1}::\left(\mathbf{1}\otimes\mathbf{1}-\mathbf{1}\overline{\underline{\otimes}}\mathbf{1}\right)=0$ stands.

Here we first aim at rewriting the constant and linear terms of the harmonic decomposition in a consistent manner with orthogonalization and notations introduced in 2D Tensorial Polar Decomposition [24]. In order to do so, instead of expression (18), we prefer to start from the (equivalent) Backus fully orthogonalized expression [5,7]

$$\mathbb{S}=r_{\mathrm{c}}\mathbf{1}\circledast\mathbf{1}+2\bar{r}_{\mathrm{c}}\left(\mathbf{1}\otimes\mathbf{1}-\mathbf{1}\overline{\underline{\otimes}}\mathbf{1}\right)+\mathbf{1}\circledast\mathbf{s}_1'+\mathbf{s}_1'\circledast\mathbf{1}+\mathbf{1}\otimes\mathbf{s}_2'+\mathbf{s}_2'\otimes\mathbf{1}-\mathbf{s}_2'\overline{\underline{\otimes}}\mathbf{1}-\mathbf{1}\overline{\underline{\otimes}}\mathbf{s}_2'+\mathbb{H} \tag{21}$$

introducing two harmonic (symmetric deviatoric) second-order tensors $\mathbf{s}_1'$ and $\mathbf{s}_2'$ related to $\boldsymbol{\alpha}'$ and $\boldsymbol{\beta}'$. We make appear moduli r_{l}, $\bar{r}_{\mathrm{l}}$ (generalizing to 3D the 2D polar modulus r_1) by defining the 3D symmetric deviatoric tensors $\mathbf{S}_{r\mathrm{l}}'$ and $\bar{\mathbf{S}}_{\bar{r}\mathrm{l}}'$ of unit norm $J_2(\mathbf{S}_{r\mathrm{l}}')=J_2(\bar{\mathbf{S}}_{\bar{r}l}')=1$ as

$$r_{\mathrm{l}}\mathbf{S}_{r\mathrm{l}}'=\mathbf{s}_1'=\boldsymbol{\alpha}'+2\boldsymbol{\beta}'=\frac{1}{7}\left(\mathbf{d}'+2\mathbf{v}'\right)\qquad \bar{r}_{\mathrm{l}}\bar{\mathbf{S}}_{\bar{r}\mathrm{l}}'=\frac{1}{2}\mathbf{s}_2'=\frac{1}{3}\left(\boldsymbol{\alpha}'-\boldsymbol{\beta}'\right)=\frac{1}{3}\left(\mathbf{d}'-\mathbf{v}'\right) \tag{22}$$

[2] $\mathrm{SO}(3)=\{\mathbf{g}\,/\,\mathbf{g}^{-1}=\mathbf{g}^{\mathrm{T}},\det\mathbf{g}=1\}$ is the group of rotations in 3D.

The tensors $r_n\mathbf{S}'_n$ generalize to 3D the 2D symmetric deviatoric tensors $r_n\mathbf{R}'_n$ of section 2. In the present work, the J_2-norm is defined as $J_2(\mathbf{X})=(\frac{1}{2}\mathbf{X}':\mathbf{X}')^{1/2}$. Eq. (22) makes appear the J_2-norms:

$$r_1=\frac{1}{7}J_2(\mathbf{d}'+2\mathbf{v}') \qquad \bar{r}_1=\frac{1}{3}J_2(\mathbf{d}'-\mathbf{v}') \tag{23}$$

As norms of tensors, the moduli r_1 and $\bar{r}_1$ are positive invariants.

We therefore start from orthogonalized harmonic decomposition of any symmetric tensor $\mathbb{S}$ rewritten as:

$$\mathbb{S}=r_c\mathbf{1}\circledast\mathbf{1}+2\bar{r}_c\left(\mathbf{1}\otimes\mathbf{1}-\mathbf{1}\,\overline{\underline{\otimes}}\,\mathbf{1}\right)+r_1\left(\mathbf{1}\circledast\mathbf{S}'_{r1}+\mathbf{S}'_{r1}\circledast\mathbf{1}\right)+2\bar{r}_1\left(\mathbf{1}\otimes\bar{\mathbf{S}}'_{\bar{r}1}+\bar{\mathbf{S}}'_{\bar{r}1}\otimes\mathbf{1}-\bar{\mathbf{S}}'_{\bar{r}1}\,\overline{\underline{\otimes}}\,\mathbf{1}-\mathbf{1}\,\overline{\underline{\otimes}}\,\bar{\mathbf{S}}'_{\bar{r}1}\right)+\mathbb{H} \tag{24}$$

Any rari-constant r_c or r_1 term is orthogonal to any anti-rari-constant $\bar{r}_c$ or $\bar{r}_1$ term, orthogonality being defined in sense of scalar product :: for fourth-order tensors. Last two scalar products

$$\mathbf{1}\circledast\mathbf{1}::\left(\mathbf{1}\circledast\mathbf{S}'_{r1}+\mathbf{S}'_{r1}\circledast\mathbf{1}\right)=\left(\mathbf{1}\otimes\mathbf{1}-\mathbf{1}\,\overline{\underline{\otimes}}\,\mathbf{1}\right)::\left(\mathbf{1}\otimes\bar{\mathbf{S}}'_{\bar{r}1}+\bar{\mathbf{S}}'_{\bar{r}1}\otimes\mathbf{1}-\bar{\mathbf{S}}'_{\bar{r}1}\,\overline{\underline{\otimes}}\,\mathbf{1}-\mathbf{1}\,\overline{\underline{\otimes}}\,\bar{\mathbf{S}}'_{\bar{r}1}\right)=0 \tag{25}$$

vanish because of $\mathbf{S}':\mathbf{1}=\operatorname{tr}\mathbf{S}'=0$. It can last be checked that harmonic tensor $\mathbb{H}$ is orthogonal to each r_c, $\bar{r}_c$, r_1, $\bar{r}_1$ term of Eq. (24).

Compared to Backus orthogonalized decomposition, note that the extension of Tensorial Polar Decomposition to 3D further makes appear two scalar invariants r_1 and $\bar{r}_1$ of fourth-order tensor $\mathbb{S}$. The extension of Tensorial Polar Decomposition to 3D also needs a decomposition of harmonic part $\mathbb{H}$ generalizing Eq. (1) to 3D. This important point is addressed in the next section.

5. 3D harmonic tensor $\mathbb{H}$ expressed by means of two symmetric deviatoric second-order tensors

If $\mathbf{h}_1$ and $\mathbf{h}_2$ are harmonic second-order tensors (symmetric and deviatoric), we define the bilinear tensorial expression

$$\begin{aligned}\mathcal{H}(\mathbf{h}_1,\mathbf{h}_2)=&\frac{1}{2}(\mathbf{h}_1\circledast\mathbf{h}_2+\mathbf{h}_2\circledast\mathbf{h}_1)+\frac{2}{35}(\mathbf{h}_1:\mathbf{h}_2)\,\mathbf{1}\circledast\mathbf{1}\\&-\frac{1}{7}\left[\mathbf{1}\circledast(\mathbf{h}_1\cdot\mathbf{h}_2+\mathbf{h}_2\cdot\mathbf{h}_1)+(\mathbf{h}_1\cdot\mathbf{h}_2+\mathbf{h}_2\cdot\mathbf{h}_1)\circledast\mathbf{1}\right]\end{aligned} \tag{26}$$

It is easily checked that it defines a family of harmonic fourth-order tensor, traceless, and rari-constant. Bilinear expression (26) extends to two independent second-order tensors $\mathbf{h}_k$ the expression obtained in [27] for the coaxial cases $\mathbf{h}_2=\mathbf{h}_1$ and $\mathbf{h}_2=(\mathbf{h}_1^2)'$. For any couple of symmetric deviatoric tensors $(\mathbf{h}_1,\mathbf{h}_2)$ the harmonic tensor $\mathcal{H}(\mathbf{h}_1,\mathbf{h}_2)$ is orthogonal – with respect to the scalar product :: for fourth-order tensors – to constant r_c, $\bar{r}_c$ terms and to linear r_1, $\bar{r}_1$ terms of the orthogonalized harmonic decomposition (24).

In order to represent $\mathbb{H}$, Böhlke and Bertram [27] have introduced three generators $\mathbb{G}^{(\alpha)}$, $\mathbb{G}^{(\beta)}$, $\mathbb{G}^{(\gamma)}$, all three built from the single-unit deviatoric tensor $\mathbf{h}=\mathbf{h}'$. The harmonic tensor $\mathbb{H}$ has been considered as the sum of three terms $\mathbb{H}=g_\alpha\,\mathbb{G}^{(\alpha)}+g_\beta\,\mathbb{G}^{(\beta)}+g_\gamma\,\mathbb{G}^{(\gamma)}$ with $g_k=g_k(\det\mathbf{h})$ functions of the only non-constant principal invariant $\det\mathbf{h}$ of $\mathbf{h}$, with $\mathbb{G}^{(\alpha)}=\mathcal{H}(\mathbf{h},\mathbf{h})$, $\mathbb{G}^{(\beta)}=\mathcal{H}((\mathbf{h}^2)',(\mathbf{h}^2)')$, $\mathbb{G}^{(\gamma)}=\mathcal{H}((\mathbf{h}^2)',\mathbf{h})$, which are function of the same harmonic tensor $\mathbf{h}$ and where the bilinear form $\mathcal{H}(.,.)$ is the one defined in Eq. (26).

Instead, we propose to define each elementary harmonic generator as a function of a *different* deviatoric second-order tensor $\mathbf{h}_k$,

$$\mathbb{G}^{(qk)}=\mathcal{H}(\mathbf{h}_k,\mathbf{h}_k)=\mathbf{h}_k\circledast\mathbf{h}_k+\frac{2}{35}(\mathbf{h}_k:\mathbf{h}_k)\,\mathbf{1}\circledast\mathbf{1}-\frac{2}{7}\left(\mathbf{1}\circledast\mathbf{h}_k^2+\mathbf{h}_k^2\circledast\mathbf{1}\right) \tag{27}$$

the upperscript q standing for "quadratic". Tensors $\mathbf{h}_k$ are chosen next to the unit J_2-norm, $J_2(\mathbf{h}_k)=1$. Each fourth-order tensor $\mathbb{G}^{(qk)}$ introduces four parameters : one invariant, the determinant $\det\mathbf{h}_k$ of the normalized deviatoric tensor $\mathbf{h}_k$, and three frame angles. We propose to describe $\mathbb{H}\in\mathbb{H}\mathrm{rm}$ as the sum $\mathbb{H}=\sum_{k=1}^{2}h_{qk}\mathbb{G}^{(qk)}$, with h_{qk} *ad hoc* moduli, with only two terms, which introduces 10 parameters (while the dimension of harmonic vector space $\mathbb{H}\mathrm{rm}$ is 9).

To sum up, we describe at this stage the harmonic fourth-order tensor $\mathbb{H}$ by the general form

$$\begin{aligned}\mathbb{H}=h_{q1}\mathbb{G}^{(q1)}+h_{q2}\mathbb{G}^{(q2)}=&\,h_{q1}\left[\mathbf{h}_1\circledast\mathbf{h}_1+\frac{2}{35}(\mathbf{h}_1:\mathbf{h}_1)\,\mathbf{1}\circledast\mathbf{1}-\frac{2}{7}\left(\mathbf{1}\circledast\mathbf{h}_1^2+\mathbf{h}_1^2\circledast\mathbf{1}\right)\right]\\&+h_{q2}\left[\mathbf{h}_2\circledast\mathbf{h}_2+\frac{2}{35}(\mathbf{h}_2:\mathbf{h}_2)\,\mathbf{1}\circledast\mathbf{1}-\frac{2}{7}\left(\mathbf{1}\circledast\mathbf{h}_2^2+\mathbf{h}_2^2\circledast\mathbf{1}\right)\right]\end{aligned} \tag{28}$$

which,

- is orthogonal to linear and constant terms, *i.e.* to the difference $\mathbb{S}-\mathbb{H}$ obtained from harmonic decomposition (18) (or from orthogonalized harmonic decomposition (24)),
- introduces 10 parameters.

If combined with an additional condition, equation (28) has nine independent parameters, i.e. as much as the dimension of the harmonic vector space $\mathbb{H}$rm. Nevertheless, we do not seek in our approach such a condition as equation (28) will leave us with a useful degree of freedom to perform the practical decomposition, see section 8. Instead we propose next a nine-parameter representation based on equation (28), which does not need any *ad hoc* condition.

When the moduli h_{q1}, h_{q2} are of opposite signs, one has, due to the symmetrization made by $\mathcal{H}(.,.)$, here with $h_{q1} > 0$:

$$\mathbb{H} = \mathcal{H}\left(\sqrt{h_{q1}}\,\mathbf{h}_1 + \sqrt{-h_{q2}}\,\mathbf{h}_2, \sqrt{h_{q1}}\,\mathbf{h}_1 - \sqrt{-h_{q2}}\,\mathbf{h}_2\right) \tag{29}$$

If $h_{q1} < 0$ and $h_{q2} > 0$, one has to simply swap the corresponding terms to enforce a novel $h_{q1} > 0$.

Let us norm such a bilinear $\mathbb{H}$ by making appear the J_2-norm of second-order tensors $\sqrt{h_{q1}}\,\mathbf{h}_1 \pm \sqrt{-h_{q2}}\,\mathbf{h}_2$ and the quadratic norm $\|\mathbb{H}\| = \sqrt{\mathbb{H} :: \mathbb{H}}$ of the harmonic tensor itself, defining symmetric deviatoric (harmonic) second-order tensors of unit J_2-norms

$$\mathbf{S}'_{rq1} = \frac{\sqrt{h_{q1}}\,\mathbf{h}_1 + \sqrt{-h_{q2}}\,\mathbf{h}_2}{J_2(\sqrt{h_{q1}}\,\mathbf{h}_1 + \sqrt{-h_{q2}}\,\mathbf{h}_2)} \qquad \mathbf{S}'_{rq2} = \frac{\sqrt{h_{q1}}\,\mathbf{h}_1 - \sqrt{-h_{q2}}\,\mathbf{h}_2}{J_2(\sqrt{h_{q1}}\,\mathbf{h}_1 - \sqrt{-h_{q2}}\,\mathbf{h}_2)} \qquad J_2(\mathbf{S}'_{rq1}) = J_2(\mathbf{S}'_{rq2}) = 1 \tag{30}$$

and defining modulus r_q as the norm of $\mathbb{H}$

$$r_q = \|\mathbb{H}\| = \left\|\mathcal{H}\left(\sqrt{h_{q1}}\,\mathbf{h}_1 + \sqrt{-h_{q2}}\,\mathbf{h}_2, \sqrt{h_{q1}}\,\mathbf{h}_1 - \sqrt{-h_{q2}}\,\mathbf{h}_2\right)\right\| \tag{31}$$

This defines r_q as a scalar invariant of the symmetric fourth-order tensor $\mathbb{S}$. One has then, using definition (26),

$$\mathbb{H} = r_q \mathbb{G}^{(q)} = r_q \frac{\mathcal{H}\left(\mathbf{S}'_{rq1}, \mathbf{S}'_{rq2}\right)}{\|\mathcal{H}\left(\mathbf{S}'_{rq1}, \mathbf{S}'_{rq2}\right)\|} \qquad \text{(no sum)} \tag{32}$$

By the proposed change of variables, the novel expression (32) now expresses the harmonic part $\mathbb{H}$ of the symmetric tensor $\mathbb{S}$ as a function of one scalar invariant (r_q, the norm of $\mathbb{H}$) and of two symmetric deviatoric second-order unit tensors ($\mathbf{S}'_{rq1}, \mathbf{S}'_{rq2}$). This expression has the nice property to directly make appear the nine independent parameters of $\mathbb{H}$ as one for modulus r_q and as two times the four parameters of symmetric deviatoric tensors $\mathbf{S}'_{rqk}$ of unit J_2-norm.

The same result (an expression with nine independent parameters) is derived when h_{q1} and h_{q2} are of the same sign, still as Eq. (32), real, but with $\mathbf{S}'_{rq1}$ replaced by the complex symmetric deviatoric second-order tensor $\mathbf{S}'_{rq}$ and with $\mathbf{S}'_{rq2}$ replaced by the complex conjugate tensor $\mathbf{S}^{\star\prime}_{rq}$, setting $i^2 = -1$ and defining the complex deviatoric symmetric second-order tensor

$$\mathbf{S}'_{rq} = \frac{\sqrt{h_{q1}}\,\mathbf{h}_1 + \mathrm{i}\sqrt{h_{q2}}\,\mathbf{h}_2}{J_2(\sqrt{h_{q1}}\,\mathbf{h}_1 + \mathrm{i}\sqrt{h_{q2}}\,\mathbf{h}_2)} \qquad J_2(\mathbf{S}'_{rq}) = J_2(\mathbf{S}^{\star\prime}_{rq}) = \sqrt{\frac{1}{2}\mathbf{S}'_{rq} : \mathbf{S}^{\star\prime}_{rq}} = 1 \tag{33}$$

Section 8 shows how to perform the proposed decomposition for monoclinic tensors.

Remark. Properties (16)–(17) imply that the action of any rotation $\mathbf{g}$ is such that[3]

$$\begin{aligned}
&\mathbf{g} \star \sum_{k=1}^{2} h_{qk}\mathcal{H}(\mathbf{h}_k, \mathbf{h}_k) = \sum_{k=1}^{2} h_{qk}\mathcal{H}(\mathbf{g}\star\mathbf{h}_k, \mathbf{g}\star\mathbf{h}_k) = \sum_{k=1}^{2} h_{qk}\mathcal{H}(\mathbf{g}\cdot\mathbf{h}_k\cdot\mathbf{g}^{\mathrm{T}}, \mathbf{g}\cdot\mathbf{h}_k\cdot\mathbf{g}^{\mathrm{T}})\\
&\mathbf{g}\star\mathcal{H}\left(\mathbf{S}'_{rq1}, \mathbf{S}'_{rq2}\right) = \mathcal{H}\left(\mathbf{g}\star\mathbf{S}'_{rq1}, \mathbf{g}\star\mathbf{S}'_{rq2}\right) = \mathcal{H}\left(\mathbf{g}\cdot\mathbf{S}'_{rq1}\cdot\mathbf{g}^{\mathrm{T}}, \mathbf{g}\cdot\mathbf{S}'_{rq2}\cdot\mathbf{g}^{\mathrm{T}}\right)\\
&\|\,\mathbf{g}\star\mathcal{H}\left(\mathbf{S}'_{rq1}, \mathbf{S}'_{rq2}\right)\| = \|\,\mathcal{H}\left(\mathbf{S}'_{rq1}, \mathbf{S}'_{rq2}\right)\|
\end{aligned} \tag{34}$$

which implies that the scalars r_q, h_{q1} and h_{q2} are frame independent.

6. Extension to antisymmetric tensors $\mathbb{A}$

Irreductible harmonic decomposition of the 3D non-symmetric fourth-order tensor $\mathbb{T} \in \mathbb{G}$el (having minor indicial symmetry only) is the decomposition [3]

$$R \oplus R \oplus V \oplus \mathbf{Dev} \oplus \mathbf{Dev} \oplus \mathbf{Dev} \oplus \mathbf{Hrm} \oplus \mathbb{H}\mathrm{rm} \tag{35}$$

[3] The action of rotation group SO(3) commutes with $\mathcal{H}$. Proposed representation of harmonic tensors is SO(3) equivariant.

of tensor $\mathbb{T}$ into two scalar invariants $\in R$, one vector $\mathrm{v} \in$ vector space V (of component v_i), three symmetric deviatoric (harmonic) second-order tensors $\in \mathbf{D}\mathrm{ev}$, one totally symmetric traceless (harmonic) third order tensor $\mathbf{H} \in \mathbf{H}\mathrm{rm}$ ($\mathrm{H}_{ijk} = \mathrm{H}_{ikj} = \mathrm{H}_{jik}$, $\mathrm{H}_{kki} = 0$) and one harmonic fourth-order tensor $\mathbb{H} \in \mathbb{H}\mathrm{rm}$. For antisymmetric part $\mathbb{A} = \frac{1}{2}(\mathbb{T} - \mathbb{T}^{\mathrm{T}})$, it is classically [3]

$$V \oplus \mathbf{D}\mathrm{ev} \oplus \mathbf{H}\mathrm{rm} \tag{36}$$

$\mathbb{A}$ is (major) antisymmetric, *i.e.* it has minor indicial symmetries $A_{ijkl} = A_{ijlk} = A_{jikl}$ and is such that $A_{ijkl} = -A_{klij}$.

A third- and a fourth-order tensors are present within the harmonic decomposition (35), a third-order tensor in Eq. (36), as irreducibility is meant in the sense of linearity of vector spaces. The harmonic fourth-order tensor $\mathbb{H}$ and the symmetric part $\mathbb{S} = \frac{1}{2}(\mathbb{T} + \mathbb{T}^{\mathrm{T}})$ have been just expressed by means of second-order tensors only (as quadratic expression (28) for harmonic term, loosing the linearity feature). In a manner similar to the case of $\mathbb{H}$, the purpose next is to derive the inner nonlinear structure of the antisymmetric fourth-order tensor $\mathbb{A}$ and of its traceless part $\mathbb{Z}$, $Z_{kkij} = Z_{kikj} = 0$, as a function of second-order tensors only, possibly antisymmetric.

6.1. Case of 2D antisymmetric tensors

In 2D, the harmonic decomposition of (major) antisymmetric tensors is $R \oplus \mathbf{D}\mathrm{ev}^{(2\mathrm{D})}$, recast from Eq. (6) as

$$\mathbb{A} = t_3 \left[\mathbf{1} \underline{\otimes} \mathbf{A} + \mathbf{A} \underline{\otimes} \mathbf{1} \right] + 2 r_3 \left(\mathbf{1} \otimes \mathbf{R}'_3 - \mathbf{R}'_3 \otimes \mathbf{1} \right) \quad \text{with} \quad \mathbf{A} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{37}$$

There is one constant term (of polar modulus t_3), and one linear term defined using one polar modulus r_3 and one second-order tensor $\mathbf{R}'_3$, which is symmetric deviatoric and of unit J_2-norm. There is no quadratic term.

6.2. Linear terms in 3D

Any 3D antisymmetric fourth-order tensor $\mathbb{A}$ having minor indicial symmetries only has two independent traces,

$$\mathbf{e}(\mathbb{A}) = \mathrm{tr}_{12}\, \mathbb{A} = -\,\mathrm{tr}_{34}\, \mathbb{A} = -\mathbf{d}(\mathbb{A}) = 3\, \mathbf{s}' \qquad \mathbf{v}(\mathbb{A}) = \mathbf{v}^{\mathrm{A}} = \mathrm{tr}_{13}\, \mathbb{A} = 5\, \mathbf{a} \tag{38}$$

where $\mathbf{v}^{\mathrm{A}} = \frac{1}{2}(\mathbf{v} - \mathbf{v}^{\mathrm{T}})$ is the antisymmetric part of the Voigt tensor $\mathbf{v} = \mathbf{v}(\mathbb{T})$ of $\mathbb{T}$. Two second-order tensors are defined: a symmetric deviatoric tensor $\mathbf{s}'$ and an antisymmetric tensor $\mathbf{a} = \mathbf{a}' = -\mathbf{a}^{\mathrm{T}}$. A rewriting of the harmonic decomposition (36) of antisymmetric tensors reads then

$$\mathbb{A} = \mathbf{1} \otimes \mathbf{s}' - \mathbf{s}' \otimes \mathbf{1} + \mathbf{1} \underline{\otimes} \mathbf{a} + \mathbf{1} \overline{\otimes} \mathbf{a} + \mathbf{a} \underline{\otimes} \mathbf{1} + \mathbf{a} \overline{\otimes} \mathbf{1} + \mathbb{Z} \tag{39}$$

with $\mathbf{1} \otimes \mathbf{s}' - \mathbf{s}' \otimes \mathbf{1}$ and $\mathbf{1} \underline{\otimes} \mathbf{a} + \mathbf{1} \overline{\otimes} \mathbf{a} + \mathbf{a} \underline{\otimes} \mathbf{1} + \mathbf{a} \overline{\otimes} \mathbf{1} = 2\,(\mathbf{1} \overline{\underline{\otimes}} \mathbf{a} + \mathbf{a} \overline{\underline{\otimes}} \mathbf{1})$, both being major antisymmetric (having minor indicial symmetry), with $\mathbb{Z}$ a major antisymmetric and traceless tensor (having minor indicial symmetry), $\mathrm{tr}_{ij}\, \mathbb{Z} = 0$, $\forall i \neq j$. As needed for an antisymmetric tensor with minor symmetries, there are 15 independent parameters introduced: five by symmetric deviatoric $\mathbf{s}'$, three by antisymmetric $\mathbf{a}$ (which is isomorphic to vector $\mathbf{v}$), and seven by $\mathbb{Z}$ (which is isomorphic to the harmonic third-order tensor $\mathbf{H}$).

Note that in 3D there is no constant term (such as the 2D term in t_3) and contrary to 2D, there is a traceless term $\mathbb{Z}$, which will be next interpreted as a quadratic term, as we did for $\mathbb{H}$ in the case of symmetric tensors.

In the same manner as for Tensorial Polar Decomposition, we now make the J_2-norms of the second-order tensors appear, setting $\mathbf{s}' = a_{\mathrm{Sl}}\, \mathbf{S}'_{\mathrm{al}}$ (symmetric deviatoric) and $\mathbf{a} = a_{\mathrm{Al}}\, \mathbf{A}_{\mathrm{al}}$ (antisymmetric) with tensors $\mathbf{S}'_{\mathrm{al}}$ and $\mathbf{A}_{\mathrm{al}}$ of unit J_2-norm. This defines scalars a_{Sl} and a_{Al} as positive invariant (frame independent) moduli,

$$a_{\mathrm{Sl}} = J_2(\mathbf{s}'), \qquad a_{\mathrm{Al}} = J_2(\mathbf{a}), \qquad J_2(\mathbf{S}'_{\mathrm{al}}) = J_2(\mathbf{A}_{\mathrm{al}}) = 1 \tag{40}$$

Subscript l means “linear term”. Subscript S for a_{Sl} and A for a_{Al} refer to the capital letter of the corresponding unit second-order tensor (either $\mathbf{S}'_{\mathrm{al}}$ or $\mathbf{A}'_{\mathrm{al}}$). Letters a stand for “antisymmetric contribution”, they recall that the fourth-order tensor $\mathbb{A}$ built with second-order tensors $a_{\mathrm{Sl}}\mathbf{S}'_{\mathrm{al}}$ and $a_{\mathrm{Al}}\mathbf{A}'_{\mathrm{al}}$ is (major) antisymmetric.

The decomposition (39) is therefore recast as

$$\mathbb{A} = a_{\mathrm{Sl}} \left(\mathbf{1} \otimes \mathbf{S}'_{\mathrm{al}} - \mathbf{S}'_{\mathrm{al}} \otimes \mathbf{1} \right) + 2 a_{\mathrm{Al}} \left(\mathbf{1} \overline{\underline{\otimes}} \mathbf{A}_{\mathrm{al}} + \mathbf{A}_{\mathrm{al}} \overline{\underline{\otimes}} \mathbf{1} \right) + \mathbb{Z} \tag{41}$$

in a form that makes appear (major) antisymmetric generators, orthogonal to any fourth-order symmetric tensor $\mathbb{S}$, orthogonal to each other,

$$\left(\mathbf{1} \otimes \mathbf{S}'_{\mathrm{al}} - \mathbf{S}'_{\mathrm{al}} \otimes \mathbf{1} \right) :: \left(\mathbf{1} \overline{\underline{\otimes}} \mathbf{A}_{\mathrm{al}} + \mathbf{A}_{\mathrm{al}} \overline{\underline{\otimes}} \mathbf{1} \right) = 0 \tag{42}$$

and orthogonal to the traceless tensor $\mathbb{Z}$ as

$$\left(\mathbf{1} \otimes \mathbf{S}'_{\mathrm{al}} - \mathbf{S}'_{\mathrm{al}} \otimes \mathbf{1} \right) :: \mathbb{Z} = \left(\mathbf{1} \overline{\underline{\otimes}} \mathbf{A}_{\mathrm{al}} + \mathbf{A}_{\mathrm{al}} \overline{\underline{\otimes}} \mathbf{1} \right) :: \mathbb{Z} = 0 \tag{43}$$

6.3. Quadratic term: the antisymmetric traceless tensor $\mathbb{Z}$

Our aim is to generalize the 2D Tensorial Polar Decomposition (Eq. (5)) to 3D non-symmetric tensors (having minor indicial symmetries only). It is to express fourth-order tensors having minor indicial symmetries by means of second-order tensors only by making orthogonal contributions appear (and related invariants), i.e. to make appear the (linear) terms that rotate as second-order tensors do and the (quadratic) terms that rotate as only fourth-order tensors can do.

The expressions for the fourth-order harmonic tensor $\mathbb{H}$ have been derived in section 5 thanks to orthogonality to constant and linear terms of the harmonic decomposition for symmetric tensors. The same derivations can be followed for $\mathbb{Z}$, starting from the property that tensor $\mathbf{S}' \overline{\underline{\otimes}}\, \mathbf{A} + \mathbf{A} \overline{\underline{\otimes}}\, \mathbf{S}'$ is antisymmetric for any symmetric deviatoric second-order tensor $\mathbf{S}'$ and any antisymmetric second-order tensor $\mathbf{A}$. A most important feature is that, with $\mathbf{S}'$ and $\mathbf{A}$, of unit norms, this is the only tensorial antisymmetric bilinear term built from tensorial products $\otimes$, $\underline{\otimes}$, $\overline{\otimes}$ between second-order tensors, which introduces exactly six parameters. The needed number of seven parameters for the tensor $\mathbb{Z}$ – equal to the dimension of the vector space of antisymmetric traceless fourth-order tensors – is recovered if a multiplicative factor (related to the quadratic norm $\|\mathbb{Z}\| = \sqrt{\mathbb{Z} :: \mathbb{Z}}$) is furthermore considered. Such a multiplicative invariant modulus a_{q} will next be taken as positive (as r_0 for 2D polar decomposition, as r_{q} for the 3D decomposition of $\mathbb{H}$).

One has the following equalities:

$$\operatorname{tr}_{12}\left(\mathbf{S}' \overline{\underline{\otimes}}\, \mathbf{A} + \mathbf{A} \overline{\underline{\otimes}}\, \mathbf{S}'\right) = -\operatorname{tr}_{34}\left(\mathbf{S}' \overline{\underline{\otimes}}\, \mathbf{A} + \mathbf{A} \overline{\underline{\otimes}}\, \mathbf{S}'\right) = \mathbf{S}' \cdot \mathbf{A} - \mathbf{A} \cdot \mathbf{S}' \tag{44}$$

$$\operatorname{tr}_{13}\left(\mathbf{S}' \overline{\underline{\otimes}}\, \mathbf{A} + \mathbf{A} \overline{\underline{\otimes}}\, \mathbf{S}'\right) = \mathbf{S}' \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{S}' \tag{45}$$

with traces 12 and 34 symmetric and opposite, and with trace 13 antisymmetric.

To get the representation of $\mathbb{Z}$ by a_{q}, $\mathbf{S}' = \mathbf{S}'_{\mathrm{aq}}$ and $\mathbf{A} = \mathbf{A}_{\mathrm{aq}}$ (subscripts q standing for quadratic and a highlighting major antisymmetry), one has then

i) to define a traceless bilinear form from the term $\mathbf{S}' \overline{\underline{\otimes}}\, \mathbf{A} + \mathbf{A} \overline{\underline{\otimes}}\, \mathbf{S}'$ (as $\operatorname{tr}_{12}\mathbb{Z} = \operatorname{tr}_{34}\mathbb{Z} = \operatorname{tr}_{13}\mathbb{Z} = 0$), *i.e.*

$$\begin{aligned} \mathcal{Z}(\mathbf{S}', \mathbf{A}) = \mathbf{S}' \overline{\underline{\otimes}}\, \mathbf{A} + \mathbf{A} \overline{\underline{\otimes}}\, \mathbf{S}' & \\ - \frac{1}{3}\left[\mathbf{1} \otimes \left(\mathbf{S}' \cdot \mathbf{A} - \mathbf{A} \cdot \mathbf{S}'\right) - \left(\mathbf{S}' \cdot \mathbf{A} - \mathbf{A} \cdot \mathbf{S}'\right) \otimes \mathbf{1}\right] & \\ - \frac{1}{5}\left[\mathbf{1} \overline{\underline{\otimes}}\left(\mathbf{S}' \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{S}'\right) + \left(\mathbf{S}' \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{S}'\right) \overline{\underline{\otimes}}\, \mathbf{1}\right] & \end{aligned} \tag{46}$$

which is effectively traceless, as $\operatorname{tr}_{ij}\mathcal{Z}(\mathbf{S}', \mathbf{A}) = 0 \ \forall i \neq j$. This expression is the antisymmetric counterpart of the bilinear expression $\mathcal{H}(\mathbf{h}'_1, \mathbf{h}'_2)$ (Eq. (26)) for traceless totally symmetric fourth-order tensors;

ii) to check that expression (46) is antisymmetric (therefore orthogonal to the fourth-order symmetric part $\mathbb{S}$): this is the case because of the symmetry of $\mathbf{S}'$ and of the antisymmetry of $\mathbf{A}$, *i.e.* the symmetry of the second-order tensor $\mathbf{S}' \cdot \mathbf{A} - \mathbf{A} \cdot \mathbf{S}'$ and the antisymmetry of the second-order tensor $\mathbf{S}' \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{S}'$;

iii) to check that expression (46) is orthogonal to the linear a_{Sl} and a_{Al} terms of decomposition (41). This is found to be the case.

If the positive scalar invariant a_{q} is set as

$$a_{\mathrm{q}} = \|\mathbb{Z}\| \tag{47}$$

the proposed general representation of the traceless antisymmetric tensor $\mathbb{Z} = a_{\mathrm{q}} \frac{\mathcal{Z}(\mathbf{S}'_{\mathrm{aq}}, \mathbf{A}_{\mathrm{aq}})}{\|\mathcal{Z}(\mathbf{S}'_{\mathrm{aq}}, \mathbf{A}_{\mathrm{aq}})\|}$ is therefore the novel expression[4]

$$\begin{aligned} \mathbb{Z} = \frac{a_{\mathrm{q}}}{\|\mathcal{Z}(\mathbf{S}'_{\mathrm{aq}}, \mathbf{A}_{\mathrm{aq}})\|} \Big\{ & \mathbf{S}'_{\mathrm{aq}} \overline{\underline{\otimes}}\, \mathbf{A}_{\mathrm{aq}} + \mathbf{A}_{\mathrm{aq}} \overline{\underline{\otimes}}\, \mathbf{S}'_{\mathrm{aq}} - \frac{1}{3}\left[\mathbf{1} \otimes \left(\mathbf{S}'_{\mathrm{aq}} \cdot \mathbf{A}_{\mathrm{aq}} - \mathbf{A}_{\mathrm{aq}} \cdot \mathbf{S}'_{\mathrm{aq}}\right) - \left(\mathbf{S}'_{\mathrm{aq}} \cdot \mathbf{A}_{\mathrm{aq}} - \mathbf{A}_{\mathrm{aq}} \cdot \mathbf{S}'_{\mathrm{aq}}\right) \otimes \mathbf{1}\right] \\ & - \frac{1}{5}\left[\mathbf{1} \overline{\underline{\otimes}}\left(\mathbf{S}'_{\mathrm{aq}} \cdot \mathbf{A}_{\mathrm{aq}} + \mathbf{A}_{\mathrm{aq}} \cdot \mathbf{S}'_{\mathrm{aq}}\right) + \left(\mathbf{S}'_{\mathrm{aq}} \cdot \mathbf{A}_{\mathrm{aq}} + \mathbf{A}_{\mathrm{aq}} \cdot \mathbf{S}'_{\mathrm{aq}}\right) \overline{\underline{\otimes}}\, \mathbf{1}\right] \Big\} \end{aligned} \tag{48}$$

introducing, as needed, seven independent parameters if $\mathbf{S}' = \mathbf{S}'_{\mathrm{aq}}$ and $\mathbf{A}' = \mathbf{A}_{\mathrm{aq}}$ are taken of unit J_2-norm, $J_2(\mathbf{S}'_{\mathrm{aq}}) = J_2(\mathbf{A}_{\mathrm{aq}}) = 1$. The subscripts q are introduced to emphasize the fact that $\mathbb{Z}$ can be interpreted as a quadratic term of decomposition (41), compared to a_{Sl} and a_{Al} terms linear with respect to the second-order tensors $\mathbf{S}'_{\mathrm{al}}$ and $\mathbf{A}_{\mathrm{al}}$.

Eq. (48) is the sought general representation of the antisymmetric traceless (possibly triclinic) fourth-order tensor $\mathbb{Z}$ by means of a scalar invariant a_{q} (its norm), of a harmonic second-order tensor $\mathbf{S}'_{\mathrm{aq}}$, and of an antisymmetric second-order tensor $\mathbf{A}_{\mathrm{aq}}$ (each second-order tensor of unit norm).

It is shown in section 8.2 how to perform the proposed decomposition for monoclinic tensors.

[4] Proposed representation of $\mathbb{Z}$ is SO(3) equivariant.

7. Summary of the proposed decomposition

Expressions (24) and (41) allow us to write tensors $\mathbb{T}$ having minor indicial symmetry only as either classical sum of a (major) symmetric tensor $\mathbb{S}$ and of a (major) antisymmetric tensor $\mathbb{A}$ or as the sum of a rari-constant tensor $\mathbb{R}$ (having all indicial symmetries), of a so-called anti-rari-constant tensor $\overline{\mathbb{R}}$ (having major symmetry) and of a (major) antisymmetric tensor $\mathbb{A}$,

$$\mathbb{T} = \mathbb{S} + \mathbb{A} = \mathbb{R} + \overline{\mathbb{R}} + \mathbb{A} \tag{49}$$

The possibly triclinic tensor $\mathbb{T}$ is expressed by means of second-order tensors only, with the following general decomposition[5]

$$\begin{aligned}
&\mathbb{R} = r_{\mathrm{c}}\mathbf{1} \circledast \mathbf{1} + r_{\mathrm{l}}\left(\mathbf{1} \circledast \mathbf{S}'_{r\mathrm{l}} + \mathbf{S}'_{r\mathrm{l}} \circledast \mathbf{1}\right) + \mathbb{H}(r_{\mathrm{q}}, \mathbf{S}'_{r\mathrm{q}1}, \mathbf{S}'_{r\mathrm{q}2}) && \left(\mathbb{H}(r_{\mathrm{q}}, \mathbf{S}'_{r\mathrm{q}1}, \mathbf{S}'_{r\mathrm{q}2}) \text{ given by Eq. (32)}\right)\\
&\overline{\mathbb{R}} = 2\bar{r}_{\mathrm{c}}\left(\mathbf{1} \otimes \mathbf{1} - \mathbf{1} \overline{\underline{\otimes}} \mathbf{1}\right) + 2\bar{r}_{\mathrm{l}}\left(\mathbf{1} \otimes \bar{\mathbf{S}}'_{\bar{r}l} + \bar{\mathbf{S}}'_{\bar{r}l} \otimes \mathbf{1} - \bar{\mathbf{S}}'_{\bar{r}l} \overline{\underline{\otimes}} \mathbf{1} - \mathbf{1} \overline{\underline{\otimes}} \bar{\mathbf{S}}'_{\bar{r}l}\right)\\
&\mathbb{A} = a_{\mathrm{Sl}}\left(\mathbf{1} \otimes \mathbf{S}'_{\mathrm{al}} - \mathbf{S}'_{\mathrm{al}} \otimes \mathbf{1}\right) + 2a_{\mathrm{Al}}\left(\mathbf{1} \overline{\underline{\otimes}} \mathbf{A}_{\mathrm{al}} + \mathbf{A}_{\mathrm{al}} \overline{\underline{\otimes}} \mathbf{1}\right) + \mathbb{Z}(a_{\mathrm{q}}, \mathbf{S}'_{\mathrm{aq}}, \mathbf{A}'_{\mathrm{aq}}) && \left(\mathbb{Z}(a_{\mathrm{q}}, \mathbf{S}'_{\mathrm{aq}}, \mathbf{A}'_{\mathrm{aq}}) \text{ given by Eq. (48)}\right)
\end{aligned} \tag{50}$$

All the second-order tensors considered are of unit J_2 norm

$$J_2(\mathbf{S}'_{r\mathrm{l}}) = J_2(\bar{\mathbf{S}}'_{\bar{r}\mathrm{l}}) = J_2(\mathbf{S}'_{r\mathrm{q}1}) = J_2(\mathbf{S}'_{r\mathrm{q}2}) = J_2(\mathbf{h}_k) = J_2(\mathbf{S}'_{\mathrm{al}}) = J_2(\mathbf{A}'_{\mathrm{al}}) = J_2(\mathbf{S}'_{\mathrm{aq}}) = J_2(\mathbf{A}'_{\mathrm{aq}}) = 1 \tag{51}$$

The correct number of 36 parameters is well introduced: 15 for the rari-constant tensor $\mathbb{R}$ (including nine for $\mathbb{H}$), six for the anti-rari-constant part $\overline{\mathbb{R}}$, fifteen for the antisymmetric tensor $\mathbb{A}$ (including seven for $\mathbb{Z}$).

The rari-constant fourth-order tensors $\mathbb{T} = \mathbb{R}$, *i.e.* the totally symmetric tensors having all indicial symmetries $R_{ikjl} = R_{ijkl}$ correspond to the case $\bar{r}_{\mathrm{c}} = \bar{r}_{\mathrm{l}} = a_{\mathrm{Sl}} = a_{\mathrm{Al}} = a_{\mathrm{q}} = 0$. The symmetric tensors $\mathbb{T} = \mathbb{S}$ correspond to the case $a_{\mathrm{Sl}} = a_{\mathrm{Al}} = a_{\mathrm{q}} = 0$ and antisymmetric fourth-order tensors $\mathbb{T} = \mathbb{A}$ to $r_{\mathrm{c}} = \bar{r}_{\mathrm{c}} = r_{\mathrm{l}} = \bar{r}_{\mathrm{l}} = r_q = 0$.

8. Practical applications to monoclinic tensors

Let us address two applications: a first one concerning the decomposition of the monoclinic symmetric Hooke elasticity tensor $\mathbb{E} = \mathbb{S}$, having both minor and major symmetries, a second one concerning monoclinic non-symmetric Pockels tensor of photo-elasticity (or elasto-optics) $\mathbb{P} = \mathbb{S} + \mathbb{A}$, having minor indicial symmetry only. Monoclinic symmetry reduces in natural anisotropy basis to 13 the number of independent elasticity parameters E_{ijkl} and to 20 the number of independent photo-elasticity parameters P_{ijkl}.

For monoclinic tensors, the decomposition in Eqs. (49)–(50) is gained first from the harmonic decomposition for constant and linear terms (Eqs. (20), (22), (23)) and second, which is a novel result, from the invert of expressions (28) and (48). In the following, we will use the six-dimensional matrix representation of fourth-order tensor $\mathbb{T}$ having minor indicial symmetry,

$$[\mathbb{T}] = \begin{bmatrix}
T_{1111} & T_{1122} & T_{1133} & T_{1123} & T_{1113} & T_{1112}\\
T_{2211} & T_{2222} & T_{2233} & T_{2223} & T_{2213} & T_{2212}\\
T_{3311} & T_{3322} & T_{3333} & T_{3323} & T_{3313} & T_{3312}\\
T_{2311} & T_{2322} & T_{2333} & T_{2323} & T_{2313} & T_{2312}\\
T_{1311} & T_{1322} & T_{1333} & T_{1323} & T_{1313} & T_{1312}\\
T_{1211} & T_{1222} & T_{1233} & T_{1223} & T_{1213} & T_{1212}
\end{bmatrix} \tag{52}$$

$[\mathbb{T}]$ is symmetric when $\mathbb{T} = \mathbb{S}$ has major indicial symmetry.

The harmonic (possibly triclinic) fourth-order tensor $\mathbb{H}$ has the following matrix representation (see [18] for its expressions for the different symmetry classes):

$$[\mathbb{H}] = \begin{bmatrix}
-(\Lambda_2 + \Lambda_3) & \Lambda_3 & \Lambda_2 & X_1 & -(Y_1 + Y_2) & Z_2\\
\Lambda_3 & -(\Lambda_1 + \Lambda_3) & \Lambda_1 & X_2 & Y_1 & -(Z_1 + Z_2)\\
\Lambda_2 & \Lambda_1 & -(\Lambda_1 + \Lambda_2) & -(X_1 + X_2) & Y_2 & Z_1\\
X_1 & X_2 & -(X_1 + X_2) & \Lambda_1 & Z_1 & Y_1\\
-(Y_1 + Y_2) & Y_1 & Y_2 & Z_1 & \Lambda_2 & X_1\\
Z_2 & -(Z_1 + Z_2) & Z_1 & Y_1 & X_1 & \Lambda_3
\end{bmatrix} \tag{53}$$

[5] Proposed decomposition of $\mathbb{T}$ is SO(3) equivariant.

The traceless antisymmetric (possibly triclinic) fourth-order tensor $\mathbb{Z}$ has the following matrix representation:

$$[\mathbb{Z}]=\begin{bmatrix} 0 & \ell_0 & -\ell_0 & -(x_1+x_2) & y_2 & z_1 \\ -\ell_0 & 0 & \ell_0 & x_1 & -(y_1+y_2) & z_2 \\ \ell_0 & -\ell_0 & 0 & x_2 & y_1 & -(z_1+z_2) \\ x_1+x_2 & -x_1 & -x_2 & 0 & z_1-z_2 & y_2-y_1 \\ -y_2 & y_1+y_2 & -y_1 & z_2-z_1 & 0 & x_1-x_2 \\ -z_1 & -z_2 & z_1+z_2 & y_1-y_2 & x_2-x_1 & 0 \end{bmatrix} \tag{54}$$

In the monoclinic case, when the normal to the single symmetry plane is direction 1:

- $\mathbb{H}$ has five independent parameters Λ_1, Λ_2, Λ_3, X_1, X_2, the other parameters vanishing ($Y_1=Y_2=Z_1=Z_2=0$),
- $\mathbb{Z}$ has three independent parameters ℓ_0, x_1, x_2, the other ones vanishing ($y_1=y_2=z_1=z_2=0$).

The cases for which the normal to the single symmetry plane are direction 2 or 3 are detailed in the Appendix.

8.1. Decomposition of $\mathbb{H}$ in the monoclinic case

Let us consider the monoclinic case when the normal to the single symmetry plane is direction 1 (see Appendix A for directions 2 or 3). Using the following parametrization for $\mathbf{h}_1$ and $\mathbf{h}_2$ within Eq. (28),

$$\mathbf{h}_1=\frac{2}{\sqrt{3}}\mathbf{Q}_1^{\mathrm{T}}\cdot\begin{pmatrix}\cos\theta_1 & 0 & 0\\ 0 & \cos(\theta_1-\frac{2\pi}{3}) & 0\\ 0 & 0 & \cos(\theta_1+\frac{2\pi}{3})\end{pmatrix}\cdot\mathbf{Q}_1 \quad \text{with}\ \mathbf{Q}_1=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\varphi_1 & -\sin\varphi_1\\ 0 & \sin\varphi_1 & \cos\varphi_1\end{pmatrix} \tag{55}$$

$$\mathbf{h}_2=\frac{2}{\sqrt{3}}\begin{pmatrix}\cos\theta_2 & 0 & 0\\ 0 & \cos(\theta_2-\frac{2\pi}{3}) & 0\\ 0 & 0 & \cos(\theta_2+\frac{2\pi}{3})\end{pmatrix} \tag{56}$$

with $\mathbf{Q}_1$ a rotation matrix of angle φ_1 around axis 1, we get a monoclinic tensor $\mathbb{H}$ of components

$$\begin{aligned}
\Lambda_1&=\frac{1}{140}\left[7\left(-10h_{q1}\sin^2\theta_1\cos 4\varphi_1+h_{q1}-4h_{q2}\right)+5h_{q1}\cos 2\theta_1+40h_{q2}\cos 2\theta_2\right]\\
\Lambda_2&=\frac{1}{35}\left[-7(h_{q1}+h_{q2})-5h_{q1}\left(\sqrt{3}\sin 2\theta_1\cos 2\varphi_1+\cos 2\theta_1\right)-5h_{q2}\left(\sqrt{3}\sin 2\theta_2+\cos 2\theta_2\right)\right]\\
\Lambda_3&=\frac{1}{35}\left[-7(h_{q1}+h_{q2})+5\sqrt{3}h_{q1}\sin 2\theta_1\cos 2\varphi_1-5h_{q1}\cos 2\theta_1+5\sqrt{3}h_{q2}\sin 2\theta_2-5h_{q2}\cos 2\theta_2\right]\\
X_1&=-\frac{1}{7}\sqrt{3}h_{q1}\sin 2\theta_1\sin 2\varphi_1\\
X_2&=\frac{2}{7}h_{q1}\sin\theta_1\sin\varphi_1\cos\varphi_1\left(\sqrt{3}\cos\theta_1-7\sin\theta_1\cos 2\varphi_1\right)\\
Y_1&=Y_2=Z_1=Z_2=0
\end{aligned}$$

Those equations are inverted at given Λ_1, Λ_2, Λ_3, X_1, X_2 in the considered monoclinic case $X_1+2X_2\neq 0$ and $X_1\neq 0$. We first determine φ_1 by solving ($X_1+2X_2\neq 0$):

$$A_3(\tan 2\varphi_1)^3+A_2(\tan 2\varphi_1)^2+A_1(\tan 2\varphi_1)+A_0=0 \tag{57}$$

with

$$\begin{cases}
A_3=(X_1+2X_2)^3\\
A_2=2(X_1+2X_2)^2\left(3\Lambda_1-4(\Lambda_2+\Lambda_3)\right)\\
A_1=(X_1+2X_2)\left(8\Lambda_1^2-33\Lambda_1(\Lambda_2+\Lambda_3)+8\Lambda_2^2-33\Lambda_2\Lambda_3+8\Lambda_3^2+4(3X_1-X_2)(4X_1+X_2)\right)\\
A_0=2\left(X_1^2(97\Lambda_1-8\Lambda_2+41\Lambda_3)-4X_1X_2(\Lambda_1+8\Lambda_2)+66\Lambda_3X_1X_2+X_2^2(17(\Lambda_2+\Lambda_3)-4\Lambda_1)\right)
\end{cases} \tag{58}$$

Being a third-order polynomial, it always has at least one real solution. Then let us determine θ_1, θ_2, h_{q1} and h_{q2} using

$$\theta_1=\arctan\left[\frac{\sqrt{3}}{7}\frac{X_1+2X_2}{X_1\cos 2\varphi_1}\right] \tag{59}$$

$$\theta_2=\arctan\left[\frac{\sqrt{3}}{7}\frac{8\Lambda_1+\Lambda_2+\Lambda_3-4(X_1+2X_2)\cot 4\varphi_1}{\Lambda_2-\Lambda_3-2X_1\cot 2\varphi_1}\right] \tag{60}$$

$$h_{q1} = -\frac{2(X_1 + 2X_2)}{\sin 4\varphi_1} - \frac{7X_1}{\sqrt{3}\sin 2\varphi_1 \tan 2\theta_1} \tag{61}$$

$$h_{q2} = \frac{2(X_1 + 2X_2)}{\tan 4\varphi_1} - \frac{8\Lambda_1 + \Lambda_2 + \Lambda_3}{2} + \frac{7}{\sqrt{3}\tan 2\theta_2}\left(\frac{X_1}{\tan 2\varphi_1} - \frac{\Lambda_2 - \Lambda_3}{2}\right) \tag{62}$$

Finally, r_q, $\mathbf{S}'_{rq1}$ and $\mathbf{S}'_{rq2}$ are obtained using Eqs. (30) and (31).

Remarks: The solution may be non-unique. Divisions by zeros occur when $X_1 = 0$ and/or when $X_1 + 2X_2 = 0$, as in orthotropy case. Closed-form formulae are also obtained in such cases, simpler; they are not given in present note.

8.2. Decomposition of $\mathbb{Z}$ in the monoclinic case

Let us consider the monoclinic case when the normal to the single symmetry plane is direction 1 (see Appendix B for directions 2 or 3). Using the following parametrization for $\mathbf{S}'_{aq}$ and $\mathbf{A}_{aq}$ within Eq. (48),

$$\mathbf{S}'_{aq} = \frac{2}{\sqrt{3}}\mathbf{Q}^{\mathrm{T}}_{aq} \cdot \begin{pmatrix} \cos\theta & 0 & 0 \\ 0 & \cos(\theta - \frac{2\pi}{3}) & 0 \\ 0 & 0 & \cos(\theta + \frac{2\pi}{3}) \end{pmatrix} \cdot \mathbf{Q}_{aq} \text{ with } \mathbf{Q}_{aq} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{pmatrix} \tag{63}$$

$$\mathbf{A}_{aq} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \tag{64}$$

Recalling Eq. (47) ($a_q = \|\mathbb{Z}\|$), we get, using the notation $z_q = \frac{a_q}{\|\mathcal{Z}(\mathbf{S}'_{aq}, \mathbf{A}_{aq})\|}$:

$$\ell_0 = \frac{2}{3} z_q \sin 2\varphi \sin\theta, \quad x_1 = z_q\left(\frac{\sqrt{3}}{5}\cos\theta - \frac{1}{3}\cos 2\varphi \sin\theta\right), \quad x_2 = z_q\left(-\frac{\sqrt{3}}{5}\cos\theta + \frac{1}{3}\cos 2\varphi \sin\theta\right) \tag{65}$$

$$y_1 = y_2 = z_1 = z_2 = 0 \tag{66}$$

These equations are solved for given ℓ_0, x_1, x_2 with $z_q > 0$ and assuming $\theta \in [0, \pi]$ and $\varphi \in [-\frac{\pi}{2}, \frac{\pi}{2}]$:

$$\varphi = \frac{1}{2}\arg\left(-(x_1 + x_2) + i\ell_0\right) \qquad \theta = \arccos\left(\frac{5}{2\sqrt{3}}\frac{x_1 - x_2}{z_q}\right) \qquad z_q = \left[\frac{9}{4}\ell_0^2 + \frac{9}{4}(x_1 + x_2)^2 + \frac{25}{12}(x_1 - x_2)^2\right]^{\frac{1}{2}} \tag{67}$$

8.3. Example 1: practical decomposition of the elastic (symmetric) monoclinic tensor

The matrix representation of the elasticity tensor for feldspar (albite, $NaAlSi_3O_8$) material is [28]:

$$[\mathbb{E}] = \begin{bmatrix} 74 & 36.4 & 39.4 & 0 & -6.6 & 0 \\ & 131 & 31 & 0 & -12.8 & 0 \\ & & 128 & 0 & -20.0 & 0 \\ & & & 17.3 & 0 & -2.5 \\ & \text{SYM} & & & 29.6 & 0 \\ & & & & & 32.0 \end{bmatrix} \text{GPa} \tag{68}$$

The corresponding moduli for constant and linear terms of symmetric decomposition (24) are:

$$r_c = 101.88 \text{ GPa} \qquad \bar{r}_c = 3.10 \text{ GPa} \qquad r_l = 17.7372 \text{ GPa} \qquad \bar{r}_l = 3.76976 \text{ GPa} \tag{69}$$

$$\mathbf{S}'_{rl} = \begin{pmatrix} -0.711981 & 0. & -0.786079 \\ 0. & 0.399483 & 0. \\ -0.786079 & 0. & 0.312499 \end{pmatrix} \qquad \bar{\mathbf{S}}'_{\bar{r}l} = \begin{pmatrix} -0.389061 & 0. & -0.910756 \\ 0. & -0.0442114 & 0. \\ -0.910756 & 0. & 0.433272 \end{pmatrix} \tag{70}$$

The harmonic part of $\mathbb{E}$ is then calculated from Eq. (24), at known linear and constant terms:

$$[\mathbb{H}] = \begin{bmatrix} -2.62286 & 1.35429 & 1.26857 & 0 & 7.34286 & 0 \\ 1.35429 & 14.9486 & -16.3029 & 0 & -1.28571 & 0 \\ 1.26857 & -16.3029 & 15.0343 & 0 & -6.05714 & 0 \\ 0 & 0 & 0 & -16.3029 & 0 & -1.28571 \\ 7.34286 & -1.28571 & -6.05714 & 0 & 1.26857 & 0 \\ 0 & 0 & 0 & -1.28571 & 0 & 1.35429 \end{bmatrix} \text{GPa} \tag{71}$$

with

$$r_q = \|\mathbb{H}\| = 49.5378 \text{ GPa} \tag{72}$$

In the present full monoclinic case, with $Y_1 \neq 0$ and $Y_1 + 2Y_2 \neq 0$, Eqs. (58) to (62) (modified using permutations of Appendix A as the normal to single symmetry plane is direction 2) allow us to determine the parameters φ_1, θ_1, θ_2, h_{q1} and h_{q2}:

$$\varphi_1 = -0.280725 \qquad \theta_1 = 1.25363 \qquad \theta_2 = -0.508315 \qquad h_{q1} = -16.4682 \text{ GPa} \qquad h_{q2} = 32.2447 \text{ GPa} \tag{73}$$

so that finally, using Eq. (30) (swapping h_{q1} and h_{q2} terms to enforce the novel condition $h_{q1} > 0$ gives one real solution),

$$\mathbf{S}'_{rq1} = \begin{pmatrix} -0.622783 & 0. & 0.312225 \\ 0. & 1.09345 & 0. \\ 0.312225 & 0. & -0.47067 \end{pmatrix} \qquad \mathbf{S}'_{rq2} = \begin{pmatrix} 0.528979 & 0. & -0.278846 \\ 0. & 0.579538 & 0. \\ -0.278846 & 0. & -1.10852 \end{pmatrix} \tag{74}$$

This completes the proposed decomposition of the symmetric elasticity tensor $\mathbb{E}$ into representation (50). Compared to the applications made in [7] (following [5]), the main novelties are Eqs. (73)–(74), *i.e.* the decomposition of the fourth-order harmonic part $\mathbb{H}$ into the two second-order tensors $\mathbf{S}'_{rq1}$ and $\mathbf{S}'_{rq2}$ (and invariant $r_q = \|\mathbb{H}\|$).

8.4. Example 2: practical decomposition of photo-elastic (non-symmetric) monoclinic tensor

Matrix representation of Pockels photo-elastic tensor for monoclinic taurine ($C_2H_7NO_3S$) material is [29]:

$$[\mathbb{P}] = \begin{bmatrix} 0.313 & 0.251 & 0.270 & 0 & -0.10 & 0 \\ 0.281 & 0.252 & 0.272 & 0 & -0.0025 & 0 \\ 0.362 & 0.275 & 0.308 & 0 & -0.003 & 0 \\ 0 & 0 & 0 & 0.0025 & 0 & -0.0056 \\ -0.014 & 0.006 & 0.0048 & 0 & 0.047 & 0 \\ 0 & 0 & 0 & 0.0024 & 0 & 0.0028 \end{bmatrix} \tag{75}$$

The corresponding decomposition moduli for the constant and linear parts are:

$$r_c = 0.302613 \qquad r_l = 0.0352709 \qquad a_{Sl} = 0.0251574 \tag{76}$$

$$\bar{r}_c = 0.0892444 \qquad \bar{r}_l = 0.00175233 \qquad a_{Al} = 0.00702 \tag{77}$$

The second-order tensors associated with the linear terms are

$$\mathbf{S}'_{rl} = \begin{pmatrix} 0.43554 & 0. & -0.687535 \\ 0. & -0.838273 & 0. \\ -0.687535 & 0. & 0.402733 \end{pmatrix} \qquad \bar{\mathbf{S}}'_{\bar{r}l} = \begin{pmatrix} -0.621396 & 0. & 0.637248 \\ 0. & -0.24095 & 0. \\ 0.637248 & 0. & 0.862346 \end{pmatrix} \tag{78}$$

$$\mathbf{S}'_{al} = \begin{pmatrix} 0.808243 & 0. & -0.677732 \\ 0. & -0.178874 & 0. \\ -0.677732 & 0. & -0.62937 \end{pmatrix} \qquad \mathbf{A}'_{al} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{79}$$

The harmonic part of $\mathbb{P}$ is then calculated from Eq. (24)

$$[\mathbb{H}] = \begin{bmatrix} -0.0203371 & -0.00560286 & 0.02594 & 0 & -0.03275 & 0 \\ -0.00560286 & 0.00852 & -0.00291714 & 0 & 0.0076 & 0 \\ 0.02594 & -0.00291714 & -0.0230229 & 0 & 0.02515 & 0 \\ 0 & 0 & 0 & -0.00291714 & 0 & 0.0076 \\ -0.03275 & 0.0076 & 0.02515 & 0 & 0.02594 & 0 \\ 0 & 0 & 0 & 0.0076 & 0 & -0.00560286 \end{bmatrix} \tag{80}$$

with

$$r_q = \|\mathbb{H}\| = 0.113165 \tag{81}$$

In the present full monoclinic case, with $Y_1 \neq 0$ and $Y_1 + 2Y_2 \neq 0$, Eqs. (58) to (62) (modified using Appendix A as the normal to the single symmetry plane is direction 2) allow us to determine the parameters φ_1, θ_1, θ_2, h_{q1} and h_{q2}:

$$\varphi_1 = 0.0500631 \qquad \theta_1 = 1.08514 \qquad \theta_2 = 0.986992 \qquad h_{q1} = -0.372171 \qquad h_{q2} = 0.33829 \tag{82}$$

so that, swapping h_{q1} and h_{q2} terms to enforce the novel condition $h_{q1} > 0$ within Eq. (30), one has

$$\mathbf{S}'_{rq1} = \begin{pmatrix} -1.15344 & 0. & -0.0453512 \\ 0. & 0.587828 & 0. \\ -0.0453512 & 0. & 0.565613 \end{pmatrix} \qquad \mathbf{S}'_{rq2} = \begin{pmatrix} 0.372696 & 0. & 0.651792 \\ 0. & 0.49994 & 0. \\ 0.651792 & 0. & -0.872635 \end{pmatrix} \tag{83}$$

The traceless antisymmetric part of $\mathbb{P}$ is then calculated from Eq. (41) for known linear terms:

$$[\mathbb{Z}] = \begin{bmatrix} 0 & 0.00983333 & -0.00983333 & 0 & -0.01191 & 0 \\ -0.00983333 & 0 & 0.00983333 & 0 & 0.0128 & 0 \\ 0.00983333 & -0.00983333 & 0 & 0 & -0.00089 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.01102 \\ 0.01191 & -0.0128 & 0.00089 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.01102 & 0 & 0 \end{bmatrix} \tag{84}$$

Eqs. (47) and (67) (modified using the permutations of Appendix B as the normal to single symmetry plane is direction 2) give

$$a_q = 0.052703 \qquad \varphi = 0.327533 \qquad \theta = 0.989546 \tag{85}$$

so that second-order tensors $\mathbf{S}'_{aq}$ and $\mathbf{A}_{aq}$ are

$$\mathbf{S}'_{aq} = \begin{pmatrix} -0.979783 & 0 & -0.509165 \\ 0 & 0.634011 & 0 \\ -0.509165 & 0 & 0.345772 \end{pmatrix} \qquad \mathbf{A}_{aq} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \tag{86}$$

This completes the proposed decomposition of the photo-elasticity non-symmetric tensor $\mathbb{P}$ into representation (50). Compared to usual harmonic decomposition [5,3], the novel Eqs. (82) to (86) use second-order tensors to decompose both traceless parts $\mathbb{H}$ and $\mathbb{Z}$.

9. Conclusion

We have proposed a tensorial representation of fourth-order tensors having minor indicial symmetries only, such as (photo)elasticity tensor, or as tangent operators encountered in mechanics of materials. For 2D tensors, the proposed representation given in Eq. (6) is simply the tensorial rewriting of polar decomposition of Verchery and Vannucci for non-symmetric tensors. It includes a refined description of 2D harmonic fourth-order tensors $\mathbb{H}$ and it is checked that their 2D antisymmetric traceless counterpart $\mathbb{Z}$ vanishes.

In the 3D case of major and minor indicial symmetries, the orthogonalized harmonic decomposition is completed by the decomposition of the fourth-order harmonic part $\mathbb{H}$, possibly triclinic, which uses one scalar invariant and two symmetric and deviatoric second-order tensors. This constitutes the generalization to 3D of the Tensorial Polar Decomposition of 2D harmonic tensors recently obtained in [24]. Each second-order tensor is of unit norm, so that the number of nine independent parameters for $\mathbb{H}$ is obtained.

In the 3D case of major indicial antisymmetry (with minor indicial symmetries), one has presented an orthogonalized decomposition by means of one symmetric deviatoric second-order tensor, of one antisymmetric second-order tensor and of an antisymmetric traceless part $\mathbb{Z}$ (playing for antisymmetric tensors the same role as the harmonic part $\mathbb{H}$ for symmetric fourth-order tensors, isomorphic to a third-order harmonic tensor). This decomposition is completed by a decomposition of the possibly triclinic traceless part $\mathbb{Z}$ as a function of one scalar invariant and of two second order tensors only, a first one symmetric deviatoric, a second one antisymmetric. Each second-order tensor is of unit norm so that the number of seven independent parameters for $\mathbb{Z}$ is obtained.

The indicial symmetries explicitly appear. They are strongly related to the orthogonality of the generators introduced. They make straightforward the decomposition $\mathbb{T} = \mathbb{R} + \overline{\mathbb{R}} + \mathbb{A}$ of a tensor having minor symmetry only as the sum of a rari-constant tensor $\mathbb{R}$ (totally symmetric, 15 parameters), of an anti-rari-constant symmetric tensor $\overline{\mathbb{R}}$ (6 parameters), and of an antisymmetric tensor $\mathbb{A}$ (15 parameters).

Finally, the proposed general decomposition is performed in the particular cases of monoclinic elasticity and of monoclinic photo-elasticity.

Appendix A. Monoclinic $\mathbb{H}$ when the normal to single symmetry plane is direction 2 or 3

One has to adapt the results of section 8.1 by permutations when the normal to the single symmetry plane is direction 2 or 3.

Normal to single symmetry plane: direction 2. The parametrization for $\mathbf{h}_1$ and $\mathbf{h}_2$ is

$$\mathbf{h}_1 = \frac{2}{\sqrt{3}}\mathbf{Q}_1^{\mathrm{T}} \cdot \begin{bmatrix} \cos(\theta_1 + \frac{2\pi}{3}) & 0 & 0 \\ 0 & \cos\theta_1 & 0 \\ 0 & 0 & \cos(\theta_1 - \frac{2\pi}{3}) \end{bmatrix} \cdot \mathbf{Q}_1 \qquad \text{with } \mathbf{Q}_1 = \begin{bmatrix} \cos\varphi_1 & 0 & -\sin\varphi_1 \\ 0 & 1 & 0 \\ \sin\varphi_1 & 0 & \cos\varphi_1 \end{bmatrix} \tag{87}$$

$$\mathbf{h}_2 = \frac{2}{\sqrt{3}} \begin{bmatrix} \cos(\theta_2 + \frac{2\pi}{3}) & 0 & 0 \\ 0 & \cos\theta_2 & 0 \\ 0 & 0 & \cos(\theta_2 - \frac{2\pi}{3}) \end{bmatrix} \tag{88}$$

which results in a solution similar to the one of section 8.1 by replacing X_1 with Y_1 and X_2 with Y_2, and by doing a circular permutation of Λ_1, Λ_2, Λ_3: $\Lambda_1 \to \Lambda_2$, $\Lambda_2 \to \Lambda_3$ and $\Lambda_3 \to \Lambda_1$.

Normal to the single symmetry plane: direction 3. The parametrization for $\mathbf{h}_1$ and $\mathbf{h}_2$ is

$$\mathbf{h}_1 = \frac{2}{\sqrt{3}} \mathbf{Q}_1^{\mathrm{T}} \cdot \begin{bmatrix} \cos(\theta_1 - \frac{2\pi}{3}) & 0 & 0 \\ 0 & \cos(\theta_1 + \frac{2\pi}{3}) & 0 \\ 0 & 0 & \cos\theta_1 \end{bmatrix} \cdot \mathbf{Q}_1 \qquad \text{with } \mathbf{Q}_1 = \begin{bmatrix} \cos\varphi_1 & -\sin\varphi_1 & 0 \\ \sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{89}$$

$$\mathbf{h}_2 = \frac{2}{\sqrt{3}} \begin{bmatrix} \cos(\theta_2 - \frac{2\pi}{3}) & 0 & 0 \\ 0 & \cos(\theta_2 + \frac{2\pi}{3}) & 0 \\ 0 & 0 & \cos\theta_2 \end{bmatrix} \tag{90}$$

which results in a solution similar to the one of section 8.1 by replacing X_1 with Z_1 and X_2 with Z_2, and by doing a circular permutation of Λ_1, Λ_2, Λ_3: $\Lambda_1 \to \Lambda_3$, $\Lambda_2 \to \Lambda_1$ and $\Lambda_3 \to \Lambda_2$.

Appendix B. Monoclinic $\mathbb{Z}$ when the normal to single symmetry plane is direction 2 or 3

One has to adapt the results of section 8.2 by permutations when the normal to the single symmetry plane is direction 2 or 3.

Normal to the single symmetry plane: direction 2. The parametrization for $\mathbf{S}'_{\mathrm{aq}}$ and $\mathbf{A}_{\mathrm{aq}}$ is

$$\mathbf{S}'_{\mathrm{aq}} = \frac{2}{\sqrt{3}} \mathbf{Q}_{\mathrm{aq}}^{\mathrm{T}} \cdot \begin{bmatrix} \cos(\theta + \frac{2\pi}{3}) & 0 & 0 \\ 0 & \cos\theta & 0 \\ 0 & 0 & \cos(\theta - \frac{2\pi}{3}) \end{bmatrix} \cdot \mathbf{Q}_{\mathrm{aq}} \qquad \text{with } \mathbf{Q}_{\mathrm{aq}} = \begin{bmatrix} \cos\varphi & 0 & -\sin\varphi \\ 0 & 1 & 0 \\ \sin\varphi & 0 & \cos\varphi \end{bmatrix} \tag{91}$$

$$\mathbf{A}_{\mathrm{aq}} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \tag{92}$$

which results in a solution similar to (67) by replacing x_1 with y_1 and x_2 with y_2.

Normal to the single symmetry plane: direction 3. The parametrization for $\mathbf{S}'_{\mathrm{aq}}$ and $\mathbf{A}_{\mathrm{aq}}$ is

$$\mathbf{S}'_{\mathrm{aq}} = \frac{2}{\sqrt{3}} \mathbf{Q}_{\mathrm{aq}}^{\mathrm{T}} \cdot \begin{bmatrix} \cos(\theta - \frac{2\pi}{3}) & 0 & 0 \\ 0 & \cos(\theta + \frac{2\pi}{3}) & 0 \\ 0 & 0 & \cos\theta \end{bmatrix} \cdot \mathbf{Q}_{\mathrm{aq}} \qquad \text{with } \mathbf{Q}_{\mathrm{aq}} = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{93}$$

$$\mathbf{A}_{\mathrm{aq}} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{94}$$

which results in a solution similar to (67) by replacing x_1 with z_1 and x_2 with z_2.

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