GEOLOGICA ULTRAIECTINA

Mededelingen van de
Faculteit Aardwetenschappen
Universiteit Utrecht

No. 159

COORDINATE FREE REPRESENTATION OF THE HIERARCHICALLY SYMMETRIC TENSOR OF RANK 4 IN DETERMINATION OF SYMMETRY

REIDAR BAERHEIM

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DE COORDINAAT-ONAFHANKELIJKE REPRESENTATIE VAN DE HIERARCHISCH SYMMETRISCHE VIERDE ORDE TENSOR TER BEPALING VAN DE SYMMETRIE

ISBN 90–5744–017–2

COORDINATE FREE REPRESENTATION OF THE HIERARCHICALLY SYMMETRIC TENSOR OF RANK 4 IN DETERMINATION OF SYMMETRY

De Coordinaat-onafhankelijke representatie van de hierarchisch symmetrische vierde orde tensor ter bepaling van de symmetrie

(met een samenvatting in het Nederlands)

PROEFSCHRIFT

TER VERKRIJGING VAN DE GRAAD VAN DOCTOR AAN DE UNIVERSITEIT UTRECHT,
OP GEZAG VAN DE RECTOR MAGNIFICUS,
PROF. DR H.O. VOORMA, INGEVOLGE HET BESLUIT VAN HET COLLEGE VAN DEKANEN IN HET OPENBAAR TE VERDEDIGEN OP 2 FEBRUARI 1998
DES NAMIDDAGS TE 14.30 UUR

DOOR

REIDAR BAERHEIM

GEBOREN OP 9 MAART 1948 TE RANDABERG, NOORWEGEN

1998

PROMOTOR: PROF. DR K. HELBIG

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The funding has been provided by Stavanger College, Royal Norwegian Council for Scientific and Industrial Research and Rogaland Research Academy.

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Preface

General theory of elasticity treats the anisotropic behaviour of media i.e. that property-dependence on spatial direction is taken care of. Examples of elastic media are rocks, building- and biological materials.

The tensor concept is the most fundamental concept in the description of elastic anisotropy. Although a tensor describes a physical property and as such is independent of coordinate systems, the tensor can be represented by components referred to a coordinate system. A vector – which is a first rank tensor – is the most familiar quantity where the components are dependent on the coordinate system. The set of components is a representation of the vector. A scalar quantity like the length of a vector is independent of the coordinate system to which the vector is referred to.

A main subject in my thesis, is a representation of the anisotropic elastic tensor by means of coordinate-free – or invariant – quantities to describe symmetry properties of the medium.

A question in elastic anisotropy is how material symmetry can be determined from the components of the elastic tensor. This is of main concern in my thesis.

In an arbitrary coordinate system an elastic tensor has 21 non-zero components. The exception is the isotropic tensor with some vanishing components in all coordinate systems and only two independent components. For ideal media with specified symmetry, there exist coordinate systems where some of the components are zero. How can a coordinate system which reduces the number of constants be determined, and what can be said about symmetry? The previous questions motivated investigating general theories which could represent a tool in solving such and related problems.

For experimentally observed tensors, there are no vanishing components due to deviation from ideal symmetry and inaccuracy in measurements. Thus there are 21 components for real media in any coordinate system.

A theory for representing elastic tensors geometrically was given in Backus (1970). The theory is based on a specified decomposition of the elastic tensor into harmonic tensors, and Maxwell multipoles are the geometrical representation of the harmonic tensor in 3-dimensional space. Harmonic decomposition is also done with different approaches by e.g. Mochizuki (1988) and Cowin (1989) (see Ch. 2).

Kelvin (1856) and Sutcliffe (1992) present decompositions of the elastic tensor by means of eigentensors and eigenstiffnesses (see Ch. 1). The concept was proposed by

Kelvin (1856), but does not appear to have been accepted at that time. It was independently discovered by Pipkin (1976), Rychlewsky (1984), Mehrabadi and Cowin (1990), and Sutcliffe(1992). A thorough discussion is given in Helbig (1994).

My work on coordinate-free representation is mainly based on Backus's theory including Maxwell multipoles. This thesis contains applications and further developments of his theory.

In the literature, the notation 'elastic tensor' is normally used for tensors of rank four and dimension three, describing real i.e., stable, media. Backus's theory, however, is valid regardless of the stability conditions. A tensor of rank four in three dimensions satisfying "elastic" symmetry is here defined as a hierarchically symmetric tensor. Stability conditions need not be satisfied.

According to the introduction of the concept 'hierarchically symmetric tensor', this concept was progressively taken into use in my work (Chapters 3, 4, 5 and 6). However in my first publication (Ch. 2) hierarchically symmetric tensors were not defined. I have kept it in my thesis as it was published, except for minor changes.

Theoretical analysis of elastic anisotropy has a much wider range of application than in earth sciences, and is presented in scientific diciplines like mathematics, physics, material sciences and biomechanics as well.

Most of my work is related to ideal media, with symmetry properties as in crystal physics. In Ch. 6 modeling of real media are performed by perturbation of tensors of ideal symmetry. Perturbation of a triclinic tensor models the inaccuracy of physical measurements.

Perturbation of a tensor of ideal higher symmetry, models deviation from ideal symmetry. Further work has to be done in applying the fundamentals to obtain tools for determine symmetry elements for experimentally determined tensors.

Chapter 1

Review of previous research

1.1 Introduction

Observations of seismic anisotropy in geophysics have been published over many years (Uhrig and van Melle (1955), Cholet and Richard (1954), Schmidt (1964), White, Martineau-Nicoletis and Monash (1983)). MacBeth and Crampin (1991) present a review of signal processing techniques where anisotropy is taken into account in exploration geophysics. Although observations have been recorded on seismic anisotropy, most of the work done is theoretical. Detailed reviews on progress in seismic anisotropy are given in the proceedings of the "International Workshop on Seismic Anisotropy (IWSA)". IWSA has been arranged seven times, the first one was in Suzdal, USSR, May 11-19, 1982. In the following the seven meetings are listed, with the references for the proceedings in brackets:

1. Suzdal, USSR, May 11-19, 1982; [Geophysical Journal of the Royal Astronomical Society, 76, 1, 1984]

2. Moscow, USSR, May 20-27, 1986; [Geophysical Journal of the Royal Astronomical Society, 91, 2, 1987]

3. Berkeley, CA, USA, May 31-June 4, 1988; [Journal of Geophysical Research, B, Solid Earth and Planets, 95, 7, 1990]

4. Edinburgh, UK, July 2-6, 1990; [Geophysical Journal International, 107, 3, 1991]

5. Banff, Canada, May 17-22, 1992; [Canadian Journal of Exploration Geophysics, 29, 1, 1993]

6. Trondheim, Norway, July 3-8, 1994; [Seismic Anisotropy, Society of Exploration Geophysicists, 1996, edited by Erling Fjær, Rune M. Holt and Jaswant S. Rathore.]

7. Miami, USA, February 19-23, 1996.

The proceedings from the last meeting is not yet published.

In 1994 Geophysics published about 25 papers which mainly dealt with anisotropy. That is about 15 % of the total number of publications in 1994 in that journal. The anisotropy articles covered different areas as; seismic processing, modeling, borehole geophysics. Most of the work done is theoretical rather than experimental. The 15 % share reflects the fact that seismic anisotropy has obtained an important status in the scientific part of exploration geophysics. Compared to the work done scientifically, still most commercial seismic techniques are based on the assumption of isotropic media.

Elastic anisotropy is not restricted to the field of earth sciences. Material sciences show applications in many fields, like for instance biomedical engineering. Methods on a more general basis are presented in physics and applied mathematics as well.

Estimation of elastic constants from acoustic measurements show very low activity with respect to number of publications. Few attempts have been made to estimate the parameters that describe the complexity of velocity anisotropy, namely the elastic constants, see e.g. Michelena (1994), Arts et al. (1991), Sena (1991), Jones and Wang (1981), Vernik and Nur (1992).

It is common to make an a priori assumption about the material symmetry or the approximate symmetry in much of the work done in elastic anisotropy, although the experimentalist does not know a priory what elastic symmetry a specimen may have. van Buskirk, Cowin and Carter (1986) presents a method for the measurement of the 21 independent elastic constants of the elastic tensor. The method requires measurement of the velocity and particle displacement for each of the three wave modes in six directions. The density is assumed to be known. The method is based on the fact that the eigenvalues of the Kelvin-Christoffel matrix is expressed via the density by the velocities, and the eigenvectors are the displacements. Hayes (1969) measures the elastic constants in a static way, i.e. without using acoustic waves. The method is based on measuring stress and deformation on laboratory specimens.

The main concern in my work consists of determination of symmetry of the elastic tensor when the coordinate system is arbitrary. Cowin and Mehrabadi (1987) give a classification of symmetry represented by normal to symmetry planes. The method is based on eigenvectors of two 2nd rank tensors derived from the elastic tensor (E_{ijkk} and E_{ikkj}), and eigenvectors of two second rank tensors which are, respectively, contraction of the elastic tensor with the a normal to a symmetry plane and an arbitrary unit vector in the symmetry plane. Necessary and sufficient conditions for a vector to be a normal to a plane of symmetry is that the vector is an eigenvector of the four 2nd rank tensors defined above. In chapters 2 and 5 eigenvectors of 2nd rank tensors derived from the elastic tensor are treated.

Representation of the elastic tensor by spherical harmonic functions is a subject in my work. A review of previous research in the field is given below. Since Maxwell multipole is a main concept in my work, a review of the development of the concept, and connection to the elastic tensor is given.

1.2 Maxwell multipoles. A review based on Maxwell (1881).

Maxwell (1881) gives a physical relation between the pole concept and Spherical Harmonics. Spherical Harmonics will be defined later.

In the following a review of some basic ideas of this relation is given. The starting point is to consider the potential from electrical charges. The electrical potential $V(\mathbf{r})$ from a charge q placed in the origin of a coordinate system is given as

$$V(\mathbf{r}) = \frac{q}{r} \tag{1.1}$$

where $\mathbf{r}$ = radius vector, and $r = \sqrt{x^2 + y^2 + z^2}$. It can be shown that (1.1) is a solution of Laplace's differential equation

$$\nabla^2 V = 0 \tag{1.2}$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. The linearity of the equation means that linear combinations of particular solutions satisfy the equation.

In the following it is shown that the potential, on the unit sphere, from different specific arrangements of electric charges is equal to the standard Spherical Harmonics.

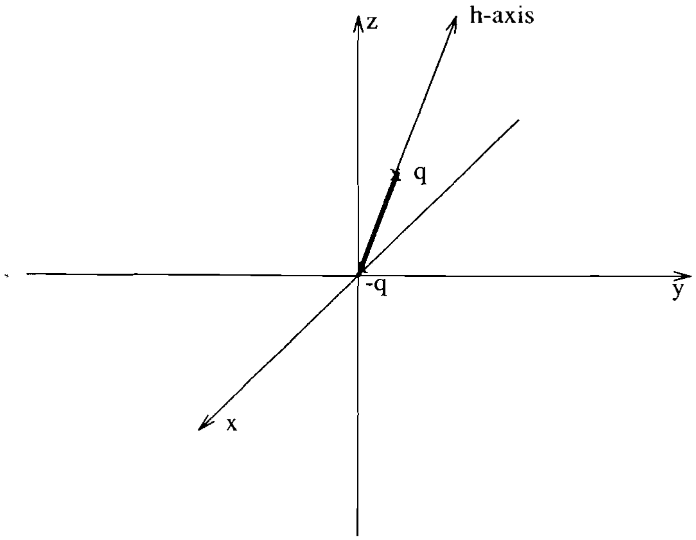

Figure 1.1: Dipole parallel to the h -axis. The h -axis defines a $\mathbf{h}$ -direction

A dipole consists of two charges q of opposite sign separated a distance h along an axis, see Fig. 1.1. In Maxwell (1881) an axis through the origin is defined by the

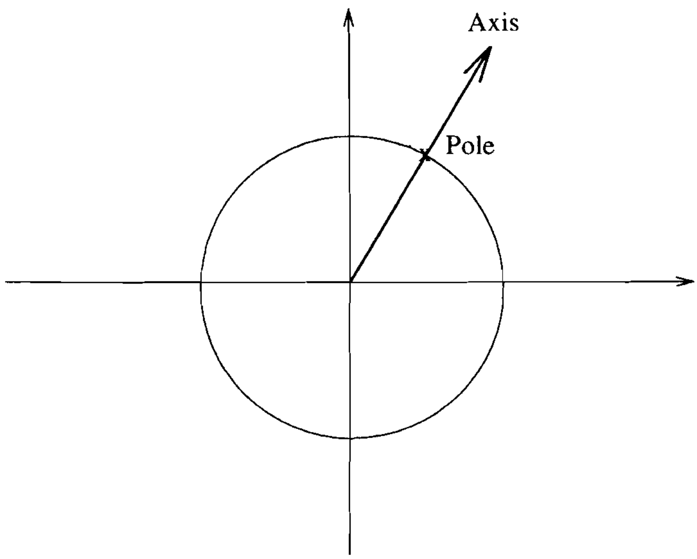

Figure 1.2: Definition of the Pole of an axis.

intersection between a sphere and a radius drawn from the center of the sphere. The intersection is called the Pole of the axis, see Fig. 1.2.

To find an expression for the potential from a dipole, let us consider the following: Let $f(\mathbf{r})$ be the potential from a charge q placed in the origin. Then $f(\mathbf{r} - h\mathbf{e}_h)$ is the potential from a charge q a distance h in the direction $\mathbf{e}_h$ where $\mathbf{e}_h$ is a unit vector in $\mathbf{h}$ -direction.

The potential from a dipole with a charge $-q$ in the origin, and q a distance h along $\mathbf{e}_h$ is then $f(\mathbf{r} - h\mathbf{e}_h) - f(\mathbf{r})$. Let h decrease and q increase but in such a way that the product qh is finite. Taylor expansion, excluding higher order terms, gives

$$f(\mathbf{r} - h\mathbf{e}_h) - f(\mathbf{r}) = -h\frac{d}{dh}f \tag{1.3}$$

Now let $\mathbf{h}_1$ denote a specified direction. From (1.1) and (1.3), we than have the following expression for the potential $V_1(\mathbf{r})$ from the dipole

$$V_1(\mathbf{r}) = -h_1\frac{d}{dh_1}V_0 = -qh_1\frac{d}{dh_1}\frac{1}{r} = qh_1\frac{\cos\delta_1}{r^2} \tag{1.4}$$

where δ_1 is the angle between $\mathbf{h}_1$ and the position vector $\mathbf{r}$. The last equality comes from the following relations:

$$\frac{d}{dh}\frac{1}{r} = -r^{-2}\frac{d}{dh}r$$

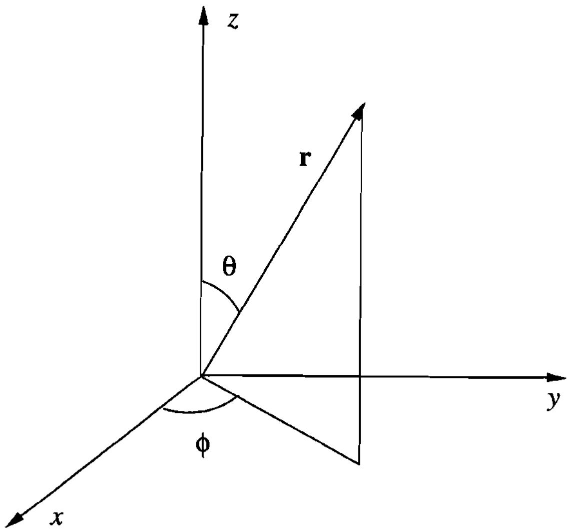

Figure 1.3: Definition of spherical coordinates ϕ and θ. r is the lenght of $\mathbf{r}$.

and

$$\frac{d}{dh}r = L\frac{\partial}{\partial x}r + M\frac{\partial}{\partial y}r + N\frac{\partial}{\partial z}r =$$

$$\frac{1}{r}(Lx + My + Nz) = \mathbf{e}_h \cdot \mathbf{e}_r = \cos\delta \tag{1.5}$$

where L, M and N are the components of $\mathbf{e}_h$. $\mathbf{e}_r$ is the unit vector in the $\mathbf{r}$ -direction.

$$\frac{d}{dh} = L\frac{\partial}{\partial x} + M\frac{\partial}{\partial y} + N\frac{\partial}{\partial z},$$

is the directional derivative operator in $\mathbf{h}$ -direction.

The potential from a dipole (equation (1.4)) becomes

$$V_1(\mathbf{r}) = A_1\frac{\cos\delta_1}{r^2} = A_1\frac{\mu_1}{r^2} \tag{1.6}$$

where $A_1 = qh_1$, and μ is defined as cosine of the angle between a $\mathbf{h}$ -axis and the position vector. When $\mathbf{h}_1$ is parallel to the z -axis, $\cos\delta = \cos\theta$, where θ is the spherical coordinate defined in Fig. 1.3

$V_1(\mathbf{r})$ in this case, $V_1^z(\mathbf{r})$, is then

$$V_1^z(\mathbf{r}) = A_1\frac{\cos\theta_1}{r^2} \propto \frac{Y_1^0(\theta,\phi)}{r^2} \tag{1.7}$$

where $Y_1^0(\theta, \phi)$ is the Surface Spherical Harmonics $Y_n^0(\theta, \phi)$ with $n = 1$. The Spherical Harmonics and the Surface Spherical Harmonics are defined in the following way: A solution $\Psi(r, \phi, \theta)$ of Laplace's equation is obtained by separation of variables $\Psi(r, \phi, \theta) = R(r)\Phi(\phi)\Theta(\theta)$, where r, ϕ and θ are the spherical coordinates. Particular homogeneous polynomial solutions of Laplace's equation for specific n is given as

$$\Psi(r, \phi, \theta) = r^n \sin(m\phi)\Theta_n^m(\theta) = r^n Y_n^{ms}(\theta, \phi) \tag{1.8}$$

and

$$\Psi(r, \phi, \theta) = r^n \cos(m\phi)\Theta_n^m(\theta) = r^n Y_n^{mc}(\theta, \phi) \tag{1.9}$$

with $mc \in \{0, 1, ..., \mathrm{n}\}$ and $ms \in \{1, ..., \mathrm{n}\}$ (see e.g. Hobson(1955)). In the literature $\Psi(r, \phi, \theta)$ are defined as the Solid Spherical Harmonics. $Y_n^{ms}(\theta, \phi)$ and $Y_n^{mc}(\theta, \phi)$ are called Surface Spherical Harmonics, and they are the Solid Spherical Harmonics on the unit sphere. $Y_n^{ms}(\theta, \phi)$ and $Y_n^{mc}(\theta, \phi)$ are linearly independent. It can been shown that if $\Psi(r, \theta, \phi) = r^n Y(\theta, \phi)$ is a solution of Laplace's equation, then also

$$\frac{\Psi(r, \theta, \phi)}{r^{2n+1}} = r^{-(n+1)} Y(\theta, \phi) \tag{1.10}$$

is a solution.

Homogeneous polynomials in three indeterminates of degree n contain $\frac{1}{2}(n+1)(n+2)$ independent terms. This is then the dimension of the vector space of homogeneous polynomials P_n,

$$\dim P_n = \frac{1}{2}(n+1)(n+2) \tag{1.11}$$

For instance when $n = 2$, the number of independent terms are 6.

Harmonic homogeneous polynomials satisfies Laplace's equation. $\nabla^2 V = 0$ produces a homogeneous expression of degree $n-2$ equated to zero (when the polynomials have degree n). From (1.11), the number of independent terms in this homogeneous expression is:

$$\frac{1}{2}(n-2+1)(n-2+2) = \frac{1}{2}(n-1)n \tag{1.12}$$

This gives $\frac{1}{2}(n-1)n$ relations between the coefficients in the original polynomial. Thus, the number of independent terms of a harmonic polynomial is:

$$\frac{1}{2}(n+1)(n+2) - \frac{1}{2}(n-1)n = 2n+1 \tag{1.13}$$

(1.8) and (1.9) constitute a set of $2n+1$ independent harmonic homogeneous polynomials in spherical coordinates (Spherical Harmonics), and thus constitute a basis for spherical harmonics of degree n. This means that any harmonic polynomial of degree n may be expressed as a linear combination of the $2n+1$ (standard) independent spherical harmonics given in (1.8) and (1.9). In the appendix a list of Spherical Harmonics up to $n = 4$ is given.

Going back to the potential V_1^z, from (1.7) we have

$$V_1^z \propto Y_1^0(\theta, \phi) \tag{1.14}$$

on the unit sphere. When the h_1 -axis is parallel to the x- and y- axes respectively, it is shown in the following that V_1 is proportional to $Y_1^{1c}(\theta, \phi)$ and $Y_1^{1s}(\theta, \phi)$ (on the unit sphere) respectively.

Generally, when the h -axis is in the xy -plane, we have

$$\mu = \sin\theta\cos(\phi - \alpha), \quad (\mu \neq 0) \tag{1.15}$$

where α is the angle of $\mathbf{h}$ relative to the x -axis.

When $\mathbf{h}_1$ is in the x -direction, $\alpha = 0$, and

$$\mu = \sin\theta\cos\phi$$

Then V_1 is given as

$$V_1^x = A_1\frac{\mu_1}{r^2} = A_1\frac{\sin\theta\cos\phi}{r^2}$$

and

$$V_1^x \propto Y_1^{1c}(\theta, \phi) \tag{1.16}$$

on the unit sphere.
When $\mathbf{h}_1$ is in the y -direction, $\alpha = \pi/2$, and

$$\mu = \sin\theta\sin\phi$$

Then we have for V_1:

$$V_1^y \propto Y_1^{1s}(\theta, \phi) \tag{1.17}$$

on the unit sphere.

A simple example of expressing a harmonic function (defined on a unit sphere) as a linear combination of standard surface spherical harmonics, is shown in the following:
Let the direction of $\mathbf{h}_1$ in the xy -plane be given by $\alpha = 2\pi/3$. Then

$$\mu = \sin\theta\cos(\phi - 2\pi/3) = \frac{1}{2}\sin\theta(\sqrt{3}\cos\phi - \sin\phi)$$

Thus, when $r = 1$,

$$V_1 = \frac{A}{2}(\sqrt{3}\sin\theta\cos\phi - \sin\theta\sin\phi) \propto$$
$$\frac{A}{2}(\sqrt{3}Y_1^{1c}(\theta, \phi) - Y_1^{1s}(\theta, \phi))$$

which is the potential associated to the direction $\mathbf{h}_1 = \cos(2\pi/3)\mathbf{e}_1 + \sin(2\pi/3)\mathbf{e}_2 = -\frac{1}{2}\mathbf{e}_1 + \frac{1}{2}\sqrt{3}\mathbf{e}_2$ in the xy -plane.

So far we have seen that each of the three spherical harmonics given by $Y_n^{ms}(\theta, \phi)$ and $Y_n^{mc}(\theta, \phi)$, for $n = 1$, corresponds to its space direction defined by (the pole of) $\mathbf{h}_1$. With $\mathbf{h}_1$ in the opposite direction, V_1 changes sign. When $\mathbf{h}_1$ is not in the direction of any coordinate axis, V_1 on the unit sphere can be expressed as a linear combination of the $Y_n^{ms}(\theta, \phi)$ and $Y_n^{mc}(\theta, \phi)$.

Summary:

To the harmonic function identical to the potential of a dipole corresponds a direction in space, defined by the (di)pole.

Maxwell calls a dipole a "point of 1st order". A point of 2nd order consists of a point of 1st order a distance h_2 along the h_2 -axis and a point of order 1 with opposite sign in the origin. The pattern of the four charges are then defined by h_1 and h_2.

The potential V_2 is obtained by

$$V_2 = -\frac{1}{2}h_2\frac{d}{dh_2}V_1 = -\frac{1}{2}h_2\frac{d}{dh_2}A_1\frac{\mu_1}{r^2} \tag{1.18}$$

where the factor $\frac{1}{2}$ is chosen for scaling purposes defined below. After some algebraic operations, we have

$$V_2 = \frac{1}{2}A_2(\frac{3\mu_1\mu_2 - \lambda_{12}}{r^3}) = \frac{1}{2}A_2(\frac{3\cos\delta_1\cos\delta_2 - \cos\epsilon_{12}}{r^3}) \tag{1.19}$$

where $A_2 = h_2A_1$ is a constant. δ is defined as above to be the angle between an h -axis and the radius vector, and ϵ_{12} is the angle between the h_1 and h_2 axes. See Fig. 1.4 for definition of symbols.

When $\mathbf{h}_1$ and $\mathbf{h}_2$ are parallel to $\mathbf{r}$,

$$\mu_1 = \mu_2 = \lambda_{12} = 1. \text{ Thus } V_2 = \frac{A_2}{r^3}$$

and has the form

$$V_n = \frac{A_n}{r^{n+1}}$$

This simple expression explains the convenience of the scaling factor $\frac{1}{2}$ above. Now consider five different arrangements of the h_1 and h_2 axes:

1). The two axes are parallel to the z -axis. In (1.19), $\lambda_{12} = 1$, and $\mu_1 = \mu_2 = \cos\theta$. V_2 then becomes

$$V_2 = \frac{1}{2}A_2(\frac{3\cos^2\theta - 1}{r^3}) \tag{1.20}$$

On the unit sphere then we have

$$V_2 \propto Y_2^0(\theta, \phi) \tag{1.21}$$

In physical applications, it is common to give $Y_n^0(\theta, \phi)$ the name: Zonal harmonics.

2). $\mathbf{h}_1$ is parallel to the z -axis, and $\mathbf{h}_2$ is parallel to the x -axis.

$$\delta_1 = \theta \Rightarrow \mu_1 = \cos\theta \qquad \alpha_2 = 0 \qquad \mu_2 = \sin\theta\cos\phi \qquad \epsilon_{12} = \pi/2$$

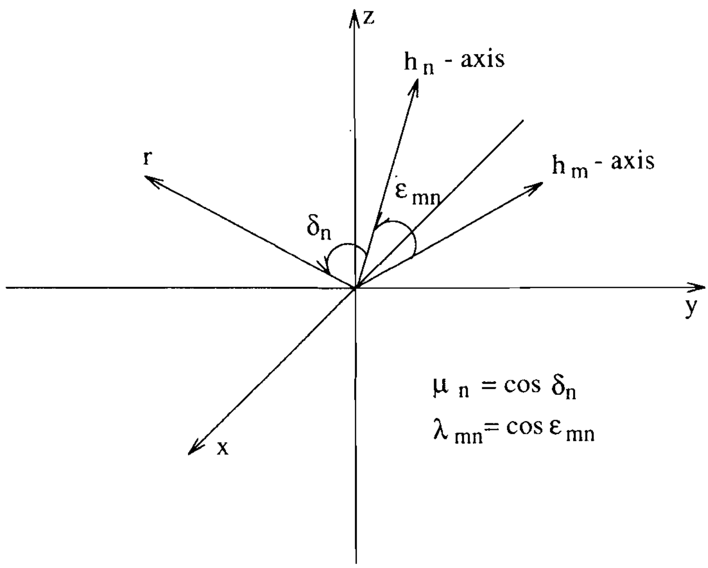

Figure 1.4: Dipole parallel to the h -axis. The h -axis defines a **h** -direction

Thus, from (1.19),

$$V_2 = \frac{3}{2} A_2 \cos\theta \sin\theta \cos\phi \propto Y_2^{1c}(\theta, \phi) \tag{1.22}$$

on the unit sphere.
Further we have:
3). $\mathbf{h}_1$ parallel to the z -axis, and $\mathbf{h}_2$ -axis parallel to the y -axis.

$$V_2 = \frac{3}{2} A_2 \cos\theta \sin\theta \sin\phi \propto Y_2^{1s}(\theta, \phi) \tag{1.23}$$

4). $\mathbf{h}_1$ and $\mathbf{h}_2$ in the $xy-$ plane. $\mathbf{h}_1$ parallel to the x -axis, and $\mathbf{h}_2$ parallel to the y -axis.

$$V_2 = \frac{3}{4} A_2 \sin^2\theta \sin 2\phi \propto Y_2^{2s}(\theta, \phi) \tag{1.24}$$

5). $\mathbf{h}_1$ and $\mathbf{h}_2$ in the $xy-$ plane. $\mathbf{h}_1$ parallel to $\cos(\pi/4)\vec{i} + \sin(\pi/4)\vec{j}$, and $\mathbf{h}_2$ parallel to $\cos(-\pi/4)\mathbf{i} + \sin(-\pi/4)\mathbf{j}$,

$$V_2(x, y, z) = -\frac{3}{4} A_2 \sin^2\theta \cos 2\phi \propto Y_2^{2c}(\theta, \phi). \tag{1.25}$$

If $\mathbf{h}_1$ and $\mathbf{h}_2$ are any other directions than the five directions specified above, the potential V_2 is a linear combination of the five standard spherical functions $Y_2^{mc}(\theta, \phi)$ and $Y_2^{ms}(\theta, \phi)$.

V_3 is the potential from a multipole characterized by three axes. It can be expressed by means of the angle between the position vector and each of the axes, and the cosine of the angle between each pair of the axes. The relation between V_3 and V_2 is, similar to the relation between V_2 and V_1, (1.18), given by

$$V_3 = -\frac{1}{3} h_3 \frac{d}{dh_3} V_2 \tag{1.26}$$

which can be written as:

$$V_3 = \frac{A_3}{2r^4}(5\mu_1\mu_2\mu_3 - (\mu_1\lambda_{23} + \mu_2\lambda_{13} + \mu_3\lambda_{12}). \tag{1.27}$$

Since V_3 do not have much relevance in the thesis, we continue to V_4. V_4 is associated to four axes, and is given by

$$V_4 = -\frac{1}{4} h_4 \frac{d}{dh_4} V_3 \tag{1.28}$$

and can be expressed as:

$$V_4 = \frac{A_4}{8r^5}\{35\mu_1\mu_2\mu_3\mu_4 - 5(\mu_1\mu_2\lambda_{34} + \mu_1\mu_3\lambda_{24} + \mu_1\mu_4\lambda_{23} + \mu_2\mu_3\lambda_{14} + \mu_2\mu_4\lambda_{13} + \mu_3\mu_4\lambda_{12}) +$$

$$+\lambda_{12}\lambda_{34} + \lambda_{13}\lambda_{24} + \lambda_{14}\lambda_{23}\} \tag{1.29}$$

When all the h -axes are parallel to $\mathbf{r}$, all μ_i and λ_{mn} are identical to 1. In that case, $V_3 = A_3/r^4$, and $V_4 = A_4/r^5$, where $A_n = h_n A_{n-1}$.
Similar to the discussion above for V_2, V_4 create the nine base spherical harmonics $Y_4^{mc}(\theta, \phi)$ and $Y_4^{ms}(\theta, \phi)$ for specific arrangements of the four associated axes.

1.3 Review of Backus (1970)

In an anisotropic material, the elastic tensor generally contains 21 nonzero components, even if the symmetry is higher than triclinic. For higher symmetry, the number of components different from zero reduces if the coordinate axes coincides with symmetry axes of the material. Backus (1970) presented a theory which is fundamental for investigating several problems in elasticity theory. The main problem focused on in this review is determination of symmetry class by means of bouquets of space directions called Maxwell multipoles. Fundamentals in Backus's theory are valid for a larger group of tensors than fourth rank tensors in three dimensions. We apply the theory to elastic tensors.

Backus defines the elastic tensor $\mathbf{E}$ as a tensor of rank four, in three dimensions, with the symmetry properties

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}. \tag{1.30}$$

The definition thus includes tensors which do not satisfy the condition of beeing positive definite, $\epsilon_{ij}\epsilon_{kl}E_{ijkl} > 0$ for all ϵ_{ij}, as well as elastic tensors describing real

media.
In later chapters (in my work), the name hierarchically symmetric tensor is used to denote a tensor of the symmetry given in (1.30), irrespective of the the stability conditions.

In the following a review of Backus's decomposition of the elastic tensor into harmonic tensors is given. Further details of Backus's theory is given in Ch. 2.
The first step in the harmonic decomposition is the splitting of the elastic tensor into the totally symmetric part **S** of the tensor **E** and the non-totally symmetric part **A**, i.e. $\mathbf{A} = \mathbf{E} - \mathbf{S}$. Backus use the name asymmetric for this remainder, in spite it has the hierarchic symmetry. The totally symmetric part of an elastic tensor, $s\mathbf{E} = \mathbf{S}$ is defined as:

$$S_{ijkl} = \frac{1}{3}(E_{ijkl} + E_{ikjl} + E_{iljk}) \tag{1.31}$$

In a totally symmetric tensor all tensor components with a specific set of indices are identical, regardless of the permutation of the indices. Harmonic tensors are defined as totally symmetric and traceless tensors. A tensor is traceless when the contraction of all pairs of two indices is zero. Harmonic tensors of a specific rank thus define a subset of elastic tensors.
The decomposition of an elastic tensor into a totally symmetric part and the remainder is:

$$\mathbf{E} = \mathbf{S} + \mathbf{A} \tag{1.32}$$

where **S** is given in (1.31). The totally symmetric part of the hierarchically symmetric tensor has 15 independent components instead of 21. The non-totally symmetric part has 6 independent components.

Each elastic tensor generates a homogeneous polynomial in three variables of degree four. The polynomial has at most 15 independent terms. This polynomial is identical to the polynomial generated by the totally symmetric part **S**, and is isomorphic to the totally symmetric part. The non-totally symmetric part of the elastic tensor is isomorphic to a (totally) symmetric tensor of rank 2 (and dimension 3).
The harmonic decomposition is performed in the following way:
1) Each of the two parts **S** and **A** is isomorphic to a homogeneous polynomial in three variables of degree four and two, respectively.
2) A homogeneous polynomial of degree $2m$ can uniquely be decomposed into harmonic polynomials of degree $2m$, $2(m-1), \ldots$. An elastic tensor is thus isomorphic to five harmonic polynomials. A harmonic polynomial of degree $2m$ is a member of the vector space of solid spherical harmonics of degree $2m$.
3) From Maxwell (1881), harmonic polynomials are isomorphic to Maxwell multipoles. To a harmonic polynomial of degree $2m$ corresponds a bouquet of $2m$ space directions called a Maxwell multipole described in the previous section, and provide a coordinate- free representation of the above five parts of the hierarchically symmetric tensor.
4) The components of Maxwell multipoles are determined from the harmonic polynomials in the following way:

- The homogeneous polynomial in three variables of degree q is mapped on a homogeneous polynomial of degree $2q$ with complex coefficients in two variables.
- A homogeneous polynomial of degree $2q$ in two variables is mapped on an inhomogeneous polynomial of degree $2q$ in one variable. The roots of these polynomials are directly related to the components of the Maxwell multipoles. There is thus a unique decomposition of an elastic tensor into harmonic tensors of rank four, two and zero.

According to Sylvester's theorem, each harmonic polynomial corresponds to a set of unit vectors and a scalar, uniquely determined except for the sign of the vectors. Thus a vector and its negative define a line, which here is defined as a direction. The bouquet of directions associated to a harmonic polynomial, determine a Maxwell multipole, (see also Maxwell (1881)). Further applications are given in Ch. 2.

1.4 Review of Cowin (1989)

Different rules for the decomposition of the elastic tensor **E** into harmonic tensors may be specified, see e.g. Cowin (1989) and Mochizuki (1988). A comparison of Backus's theory with Cowins's (1989) decomposition is given in Ch. 2. Backus's decomposition is in this article expressed by means of the Voigt tensor, the dilatational stiffness tensor and the traces of those two. Uniqueness of the decompositions is especially discussed. Cowin presents a decomposition of the elastic tensor into the same kind of harmonic tensors as Backus. Both decompositions are unique, though they are different. A comparison is given in Ch. 2 where the uniqueness problem is discussed.

In Backus (1970) each elastic tensor is expressed in terms of unique harmonic tensors, one of order 4, two of order 2 and two of order 0. But does this mean that it is the only way of decomposing **E** into harmonic tensors? Cowin shows a different decomposition into the same kind of harmonic tensors.

As in Backus's decomposition, in Cowin (1989) the elastic tensor **E** is decomposed in one fourth rank harmonic tensor, two 2nd rank harmonic tensors and two scalars. The two 2nd rank harmonic tensors are expressed by means of the deviatoric part of the dilatational- and the Voigt stiffness tensors. The two scalars are expressed by means of the traces of the dilatational- and the Voigt stiffness tensors. However, the harmonic tensors are not the same in Backus's and Cowins decompositons. Backus's harmonic decomposition is based on the decomposition of the elastic tensor into the totally symmetric part and the non-totally symmetric part of the tensor. Cowins decomposition is not based on the same, and should thus not be expected to be identical to the harmonic tensors as the harmonic tensors in Backus's decomposition.

Uniqueness of the decompositions is specially discussed in Ch. 2. Both decompositions are said to be unique, and they are, but under different assumptions. In Cowin (1989) an incorrect definition of the totally symmetric part of the elastic tensor is given, but corrected in the Corrigendum (1993) of Cowin (1989).

1.5 Spectral decomposition of the elasticity tensor.

In Sutcliffe (1992) the elastic tensor **C** is regarded as a symmetric linear transformation on the space of 2nd rank tensors. In the following a review of the theoretical part of spectral decomposition in Sutcliffe is given.

The space of 2nd rank tensors is decomposed into a subspace of symmetric tensors and subspace of skew (anti) symmetric tensors. The space of skew symmetric tensors is mapped by the elasticity tensors to the null space (see below). Thus the elastic tensor maps the space of symmetric tensors onto itself. The well known relation between stress S_{ij} and strain E_{kl} can be written as

$$S_{ij} = C_{ijkl}E_{kl} \tag{1.33}$$

where **C** is the elastic tensor.

The fact that **C** maps skew symmetric tensors **A** to zero, is easily seen from (1.33):

$$S_{ij} = C_{ijkl}A_{kl} = \frac{1}{2}C_{ijkl}(T_{kl} - T_{lk}) \tag{1.34}$$

where T_{kl} is the components of a 2nd rank tensor, and A_{kl} is the skew part of T_{kl}. Further:

$$C_{ijkl}A_{kl} = \frac{1}{2}(C_{ijkl}T_{kl} - C_{ijkl}T_{lk})$$

$$= \frac{1}{2}(C_{ij11}T_{11} - C_{ij11}T_{11} + C_{ij12}T_{12} - C_{ij12}T_{21} + C_{ij13}T_{13} - C_{ij13}T_{31}$$
$$+C_{ij21}T_{21} - C_{ij21}T_{12} + \ ...)$$

and since $C_{ijkl} = C_{ijlk}$, all terms pairwise cancel. Thus

$$C_{ijkl}A_{kl} = 0.$$

The elastic tensor maps a symmetric tensor of rank two into a symmetric tensor of rank two. Thus **C** is a mapping from the space of symmetric 2nd rank tensors to the space of symmetric 2nd rank tensors. **C** maps each strain tensor to a stress tensor. To each stress tensor also corresponds a strain tensor. Thus the mapping is onto. The dimension of the vector space of symmetric 2nd rank tensors is six.

According to the definition of tensor product of the vectors **a** and **b** (see Gurtin (1972)) we have

$$(\mathbf{a} \otimes \mathbf{b})\mathbf{u} = \mathbf{a}(\mathbf{b} \cdot \mathbf{u}) = \mathbf{a}(b_j u_j). \tag{1.35}$$

The components of the tensor product $\mathbf{a} \otimes \mathbf{b}$ relative a specific basis is then

$$(\mathbf{a} \otimes \mathbf{b})_{ij} = a_i b_j \tag{1.36}$$

As an example, let $\mathbf{n}^{(k)}$ be a unit eigenvector of a linear transformation. According to (1.35) $(\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)})\mathbf{u}$ thus is the projection of **u** in the $\mathbf{n}^{(k)}$ -direction:

$$(\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)})\mathbf{u} = \mathbf{n}^{(k)}(\mathbf{n}^{(k)} \cdot \mathbf{u}) \quad \text{no summation over } k \tag{1.37}$$

Let

$$\mathbf{u} = \alpha_k \mathbf{n}^{(k)} \quad \text{summation over } k \tag{1.38}$$

be a vector expressed as a linear combination of the orthonormal eigenvectors of a linear transformation $\mathbf{A}$ (representing a tensor) on an N dimensional vector space. The summation over k is from 1 to N. The m -th coefficient α_m is then given as

$$\alpha_m = \mathbf{u} \cdot \mathbf{n}^{(m)} \tag{1.39}$$

and by (1.37):

$$(\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)})\mathbf{u} = \alpha_k \mathbf{n}^{(k)} \tag{1.40}$$

If $\mathbf{n}^{(k)}$ is the eigenvector corresponding to the eigenvalue λ_k, we have by applying (1.38) and (1.40):

$$\mathbf{A}\mathbf{u} = \alpha_k \mathbf{A}\mathbf{n}^{(k)} = \alpha_k \lambda_k \mathbf{n}^{(k)} = \lambda_k (\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)})\mathbf{u} \quad \text{summation over } k, \quad k = 1, N \tag{1.41}$$

$\mathbf{A}$ can then be decomposed by means of spectral decomposition:

$$\mathbf{A} = \lambda_k (\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)}) \quad \text{summation over } k, \quad k = 1, N \tag{1.42}$$

If $\mathbf{A}$ is the 6×6 matrix representing the elastic tensor $\mathbf{C}$, $N = 6$, and there are six eigenvectors $\mathbf{n}^{(k)}$:

$$\mathbf{C} = \lambda_k (\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)}) \quad \text{summation over } k, \quad k = 1, 6 \tag{1.43}$$

An eigenvector in six dimension of the elastic tensor, represented as a 2nd rank tensor in three dimensions, is called an eigentensor. The six normalized eigentensors and the six eigenvalues (eigenstiffnesses) contain the 21 independent components defining the elastic tensor (see also Helbig (1994)). In Backus's decomposition, the elastic tensor is decomposed into five harmonic tensors expressed explicitly by the elastic stiffnesses. In Sutcliffe the general expression of the eigenvectors and eigentensors are not given. Thus the six tensors which compose the elastic tensor are not given explicitly.

The theory and application of eigentensors and eigenvalues (eigenstiffness) is treated in Helbig (1994). The theory is mainly based on the following papers: Kelvin (1856, 1878), Mehrabadi and Cowin (1990), Pipkin (1976) and Rychlewski (1884).

In Mehrabadi and Cowin(1990) the decomposition of the elastic tensor by means of eigenvalues and eigentensors are given for different elastic symmetries. A discussion of invariants is given as well. One important application of the theory is that it gives a tool for classifying symmetry of an elastic tensor when the coordinate system is not a natural symmetry system of the material. Comparison between Backus's decomposition and spectral decomposition remain to be done.

Chapter 2

Harmonic decomposition of the anisotropic elastic tensor

Abstract

Backus (*Rev. Geophys. Space Phys.* **8** (1970) 633) presents a theory on decomposition of the elasticity tensor and its application in several problems in anisotropy. The theory is supposed to be relatively difficult. In this article, an illustration of the theory by examples is presented. Special attention is paid to the problem of deciding which kind of symmetry a material has when the elastic constants are measured relative to an arbitrary coordinate system. A second-order symmetric tensor associated to the elasticity tensor can be used to verify if the coordinate axes are the symmetry axes of the medium, and determine a symmetry coordinate system. Also a comparison of Backus's theory with Cowin's decomposition (*Q. Jl Mech. appl. Math.* **42** (1989) 249) is presented. Uniqueness of the decompositions is specially discussed. Backus's decomposition is expressed here by means of the Voigt tensor, the dilatational modulus tensor and the traces of those two. Some misprints in Backus's expressions are indicated.

2.1 Introduction

In an anisotropic material, the elasticity tensor generally contains 21 non-zero constants. When the material has some kind of symmetry, as for instance orthorhombic or trigonal, the number of non-zero constants is reduced if the coordinate axes coincide with symmetry axes for the material.

This chapter has been published as:
Reidar Baerheim, *Harmonic decomposition of the anisotropic elasticity tensor* Q. Jl Mech. appl. Math., Vol. 46, Pt. 3, 1993

Backus (**1**) presents a theory which is fundamental for investigating several problems in elasticity theory. The theory is for instance applicable to the problem of deciding which kind of symmetry a material has when the coordinate axes are arbitrary. It is also possible from his theory to find the form of the elasticity tensor when the coordinate axes are symmetry axes. In his general theory, tensors of order q and dimension N are considered.

One purpose of this article is to give details of the computations, and to illustrate the theory by examples. The purpose is also to give applications for the elastic case where $q = 4$, and $N = 3$. A couple of errors in Backus's article will be indicated.

Important in Backus's theory is the decomposition of a fourth order tensor into one fourth order harmonic tensor, two second order tensors, and two scalars. Harmonic tensors will be defined later. Numerical examples will be shown when dealing with the elasticity tensor and its decomposition. It is also shown how the decomposition can be used to decide which kind of symmetry the material has.

This article is intended to give a better understanding of what the theory means in the elastic case where the order of the tensor is 4, the dimension is 3 and the normal elasticity relations between the tensor components are used. Also Cowin (**2**) presents a decomposition of the elasticity tensor. A comparison is given here; also uniqueness is discussed. It will be shown that there is no discrepancy between the two decompositions.

Cowin presents theorems and their proofs where the decomposition is used. One of the theorems gives the conditions for a spatial direction to be both a specific direction and a specific axis. A specific direction is a direction in which a pure longitudinal wave may propagate in an anisotropic elastic material. A specific axis is a pure shear amplitude axis, an axis about which it is possible to propagate a pure shear wave in any perpendicular direction with an amplitude lying along the axis.

The harmonic decomposition is also used by Cowin in proving the following theorem: *A necessary and sufficient condition that a vector is normal to a plane of symmetry is that it is a specific direction and a specific axis.*

2.2 Definition of a tensor

The well-known linear relation between the stress tensor σ_{ij} and the strain tensor ϵ_{kl} is the generalized Hooke's law

$$\sigma_{ij} = C_{ijkl}\,\epsilon_{kl},$$

where C_{ijkl} is the elasticity tensor, σ_{ij} and ϵ_{kl} are second-order tensors, and C_{ijkl} is of fourth order. Each of the indices i, j, k and l takes all the values 1, 2, and 3. The tensors are therefore of dimension 3.

Generally, a fourth-order tensor of dimension 3 has $3^4 = 81$ components, but the symmetry relations which are valid for the elasticity tensor reduce the number of components to 21. We study this in more detail later.

Consider now another example of a tensor. A tensor of order 1 is a vector. The vector is specified by its length and direction, and is represented by a set of three components (a_1, a_2, a_3) in a 3-dimensional space. In a new coordinate system, the vector is represented by a new set of components (a'_1, a'_2, a'_3). The set of three components is thus a representation of the vector, and the representation is related to the coordinate system.

For an array to qualify as a tensor, its components must transform from one orthonormal coordinate system to another by the rule

$$T'_{i_1 i_2 \ldots} = \alpha_{i_1 k_1} \alpha_{i_2 k_2} \ldots T_{k_1 k_2 \cdots}, \tag{2.1}$$

where $\alpha_{i_v k_v}$ is the cosine between the new i_v-axis and the old k_v-axis. See Nye **(3)** or Musgrave **(4)** for a more detailed discussion.

As we have seen, the components of a tensor are related to a specific coordinate system. In the following, we shall present a more formal definition of a tensor. With this definition, the tensor is independent of the coordinate system.

Any multilinear function $\mathbf{T}$ which assigns to every ordered q-tuple of vectors $(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_q)$ from the N-dimensional Euclidean vector space a real number $\mathbf{T}(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_q)$ will be called a qth-order functional on V_N. Such a functional is multilinear if it is linear separately in each of the q argument vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_q$. We shall see an example of this in EXAMPLE 1. By a tensor of order $q \geq 1$ over V_N we mean a qth-order functional on V_N. By this definition, the tensor is invariant under all orthogonal transformations **(5)**.

Let $\mathbf{T}$ be a tensor of order q over V_N, and let $\mathbf{e}_1, \ldots, \mathbf{e}_N$ be any orthonormal basis in V_N. If we have q vectors from V_N it follows that $\mathbf{v}_\mu = v_\mu^{(1)}\mathbf{e}_1 + v_\mu^{(2)}\mathbf{e}_2 + \cdots + v_\mu^{(N)}\mathbf{e}_N$ for $\mu = 1, \ldots, q$. By using the property of multilinearity, it follows that

$$\mathbf{T}(\mathbf{v}_1, \ldots, \mathbf{v}_q) = v_1^{(i_1)} \ldots v_q^{(i_q)} \mathbf{T}(\mathbf{e}_{i_1}, \ldots, \mathbf{e}_{i_q}), \tag{2.2}$$

$i_1, \ldots, i_q$ all run from 1 to N. The array $T_{i_1}, \ldots, T_{i_q} = \mathbf{T}(\mathbf{e}_{i_1}, \ldots, \mathbf{e}_{i_q})$ of N^q numbers is the array of components of $\mathbf{T}$ relative to the orthonormal basis. We shall also use the notation $T_{ijk\cdots} = \mathbf{T}(\mathbf{e}_i, \mathbf{e}_j, \mathbf{e}_k, \ldots)$. The representation $\mathbf{T}(\mathbf{e}_{i_1}, \ldots, \mathbf{e}_{i_q})$ is dependent of the coordinate system, and it can be shown that it transforms according to (2.1).

Further in this article, a tensor $\mathbf{T}$ will mean the representation $T_{i_1}, \ldots, T_{i_q}$ relative to a basis.

EXAMPLE 1. We shall now show how the property of multilinearity leads to a formula like (2.2) for the case when $N = 3$, and $q = 2$. Let $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ be any orthonormal basis in V_N. We can then write $\mathbf{v}_1$ and $\mathbf{v}_2$ as $\mathbf{v}_\mu = v_\mu^{(1)}\mathbf{e}_1 + v_\mu^{(2)}\mathbf{e}_2 + v_\mu^{(3)}\mathbf{e}_3$, $\mu = 1, 2$, or shortly $\mathbf{v}_\mu = v_\mu^{(i_\nu)}\mathbf{e}_{i_\nu}$ for $i_\nu = 1, 2, 3$. Then we have

$$\begin{aligned}
\mathbf{T}(\mathbf{v}_1, \mathbf{v}_2) &= \mathbf{T}(v_1^{(1)}\mathbf{e}_1 + v_1^{(2)}\mathbf{e}_2 + v_1^{(3)}\mathbf{e}_3,\ v_2^{(1)}\mathbf{e}_1 + v_2^{(2)}\mathbf{e}_2 + v_2^{(3)}\mathbf{e}_3) \\
&= v_1^{(1)}v_2^{(1)}\mathbf{T}(\mathbf{e}_1, \mathbf{e}_1) + v_1^{(1)}v_2^{(2)}\mathbf{T}(\mathbf{e}_1, \mathbf{e}_2) + v_1^{(1)}v_2^{(3)}\mathbf{T}(\mathbf{e}_1, \mathbf{e}_3) \\
&\quad + v_1^{(2)}v_2^{(1)}\mathbf{T}(\mathbf{e}_2, \mathbf{e}_1) + v_1^{(2)}v_2^{(2)}\mathbf{T}(\mathbf{e}_2, \mathbf{e}_2) + v_1^{(2)}v_2^{(3)}\mathbf{T}(\mathbf{e}_2, \mathbf{e}_3)
\end{aligned}$$

$$+v_1^{(3)}v_2^{(1)}\mathbf{T}(\mathbf{e}_3,\mathbf{e}_1)+v_1^{(3)}v_2^{(2)}\mathbf{T}(\mathbf{e}_3,\mathbf{e}_2)+v_1^{(3)}v_2^{(3)}\mathbf{T}(\mathbf{e}_3,\mathbf{e}_3)$$

using multilinearity. The array $\mathbf{T}(\mathbf{e}_{i_1},\mathbf{e}_{i_2})$ has $N^q = 3^2$ elements. According to normal convention, the above expression can be written in the same form as (2.2) as

$$\mathbf{T}(\mathbf{v}_1,\mathbf{v}_2)=v_1^{(i_1)}v_2^{(i_2)}\mathbf{T}(\mathbf{e}_{i_1},\mathbf{e}_{i_2}).$$

2.3 The homogeneous polynomial generated by a tensor

Setting $\mathbf{v}_1=\mathbf{v}_2=\cdots=\mathbf{v}_q=\mathbf{r}$ in equation (2.2) gives

$$\mathbf{T}(\mathbf{r})=r_{i_1}r_{i_2}\ldots r_{i_q}\mathbf{T}(\mathbf{e}_{i_1},\ldots,\mathbf{e}_{i_q}), \tag{2.3}$$

where $\mathbf{T}(\mathbf{r})$ is defined as $\mathbf{T}(\mathbf{r},\mathbf{r},\ldots,\mathbf{r})$ ($\mathbf{r}$ occurs q times). The $r_{i_1},r_{i_2},\ldots,r_{i_q}$ are the components of $\mathbf{r}$ relative to the basis $\mathbf{e}_1,\mathbf{e}_2,\ldots,\mathbf{e}_N$, and $i_1,i_2,\ldots,i_q$ all run from 1 to N. The expansion of $\mathbf{T}(\mathbf{r})$ from (2.3) is

$$\begin{aligned}\mathbf{T}(\mathbf{r})&=r_1r_1\ldots r_1\mathbf{T}(\mathbf{e}_1,\mathbf{e}_1,\ldots,\mathbf{e}_1)+r_1r_1\ldots r_1r_2\mathbf{T}(\mathbf{e}_1,\mathbf{e}_1,\ldots,\mathbf{e}_1,\mathbf{e}_2)+\cdots\\&+r_1r_1\ldots r_1r_N\mathbf{T}(\mathbf{e}_1,\mathbf{e}_1,\ldots,\mathbf{e}_1,\mathbf{e}_N)+r_1r_1\ldots r_2r_1\mathbf{T}(\mathbf{e}_1,\mathbf{e}_1,\ldots,\mathbf{e}_2,\mathbf{e}_1)+\\&+r_1r_1\ldots r_2r_2\mathbf{T}(\mathbf{e}_1,\mathbf{e}_1,\ldots,\mathbf{e}_2,\mathbf{e}_2)+\ldots+r_N\ldots r_N\mathbf{T}(\mathbf{e}_N,\ldots,\mathbf{e}_N)\\&=r_1^q\mathbf{T}(\mathbf{e}_1,\ldots,\mathbf{e}_1)+r_1^{q-1}r_2\mathbf{T}(\mathbf{e}_1,\ldots,\mathbf{e}_1,\mathbf{e}_2)+\cdots,\end{aligned}$$

and we see that $\mathbf{T}(\mathbf{r})$ is a homogeneous polynomial in the coordinates where the tensor-components are the coefficients. In example 1, set $\mathbf{v}_1=\mathbf{v}_2=\mathbf{r}$, and let the components of $\mathbf{r}$ relative to the basis $\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3$ be x,y, and z respectively. The result is

$$\begin{aligned}\mathbf{T}(\mathbf{r})&=x^2\mathbf{T}(\mathbf{e}_1,\mathbf{e}_1)+xy\mathbf{T}(\mathbf{e}_1,\mathbf{e}_2),+xz\mathbf{T}(\mathbf{e}_1,\mathbf{e}_3)\\&+xy\mathbf{T}(\mathbf{e}_2,\mathbf{e}_1)+y^2\mathbf{T}(\mathbf{e}_2,\mathbf{e}_2)+yz\mathbf{T}(\mathbf{e}_2,\mathbf{e}_3)\\&+xz\mathbf{T}(\mathbf{e}_3,\mathbf{e}_1)+yz\mathbf{T}(\mathbf{e}_3,\mathbf{e}_2)+z^2\mathbf{T}(\mathbf{e}_3,\mathbf{e}_3).\end{aligned}$$

The above example is also an application of (2.3). The number of different monomials, x^2, xy etc. in this example is six. This is also the dimension of the vector space consisting of all second-order homogeneous polynomials when $N=3$. Notice that the nine components of the tensor are generally different.

Generally, if $\mathbf{T}$ is a tensor of order q over V_N, then $\mathbf{T}(\mathbf{r})$ is the homogeneous polynomial of degree q generated by the tensor $\mathbf{T}$. The linear space of all homogeneous polynomials of degree q and dimension N we denote by P_N^q. Its dimension is equal to the number of different monomials in the polynomial,

$$\text{Dimension } P_N^q=\frac{(N+q-1)!}{(N-1)!q!}.$$

When $q = 4$ and $N = 3$, the dimension is 15.

EXAMPLE 2. The polynomial generated by the tensor $\mathbf{T}$ of order 4 and dimension 3 is from (2.3)

$$\begin{aligned}\mathbf{T}(\mathbf{r}) = x^4T_{1111} + x^3yT_{1112} + x^3zT_{1113} + x^3yT_{1121} + x^2y^2T_{1122} + x^2yzT_{1123} \\ +x^3zT_{1131} + x^2yzT_{1132} + x^2z^2T_{1133} + x^3yT_{1211} + x^2y^2T_{1212} \\ + \cdots + z^4T_{3333}.\end{aligned}$$

There are $3^4 = 81$ addends altogether, and by contracting coefficients with equal monomials we have

$$\begin{aligned}\mathbf{T}(\mathbf{r}) = x^4T_{1111} + x^3y(T_{1112} + T_{1121} + T_{1211} + T_{2111}) \\ +x^3z(T_{1113} + T_{1131} + T_{1311} + T_{3111}) \\ +x^2y^2(T_{1122} + T_{2211} + T_{1212} + T_{1221} + T_{2121} + T_{2112}) + \cdots \\ +xyz^2(T_{1233} + T_{1323} + T_{1332} + T_{2313} + T_{2331} + T_{3123} + T_{3132} \\ T_{2133} + T_{3213} + T_{3321} + T_{3312} + T_{3231}) + \cdots + z^4T_{3333}.\end{aligned} \tag{2.4}$$

There are 15 different monomials when $q = 4$ and $N = 3$, in accordance with the formula for the dimension of P_N^q. We shall come back to this example later.

In summary, the dimension of the vector space of all fourth-order tensors over V_3 is $3^4 = 81$; the homogeneous polynomial generated by a tensor of order 4 and dimension 3 consists of 15 different monomials; and the dimension of the vector space of all polynomials specified above is also 15.

2.3.1 Product of two tensors

If $\mathbf{S}$ and $\mathbf{T}$ are tensors of dimension N, and of order p and q respectively, the tensor product $\mathbf{ST}$ is defined as the tensor of order $p+q$ such that

$$(ST)_{i_1,\dots,i_p,j_1,\dots,j_q} = S_{i_1,\dots,i_p}T_{j_1,\dots,j_q}.$$

The generated homogeneous polynomial is then $\mathbf{S}(\mathbf{r}) \cdot \mathbf{T}(\mathbf{r})$.

EXAMPLE 3. Let $\mathbf{S}$ be a tensor of order 3, and $\mathbf{T}$ a tensor of order 2. The dimension is 3, and $\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{e}_3$ is the basis. The product of the two generated polynomials is

$$\begin{aligned}\mathbf{S}(\mathbf{r}) \cdot \mathbf{T}(\mathbf{r}) &= [x^3S_{111} + x^2yS_{112} + x^2zS_{113} + x^2yS_{121} + \cdots] \\ &\quad\times[x^2T_{11} + xyT_{12} + xzT_{13} + xyT_{21} + \cdots] \\ &= x^5S_{111}T_{11} + x^4yS_{111}T_{12} + x^4zS_{111}T_{13} + \cdots \\ &\quad +x^4yS_{112}T_{11} + x^3y^2S_{112}T_{12} + \cdots .\end{aligned}$$

There are $3^3 \times 3^2 = 3^5$ addends altogether, and so N^{p+q} terms in the polynomial generated by the tensor product. Each term of $\mathbf{T}$ is multiplied by each term of $\mathbf{S}$ to give the components in the tensor product.

2.4 Totally symmetric tensors

The number of permutations of q ordered elements is $q!$. Let π denote a change of the q ordered elements into a permutation, and let πi denote the element which replaces i in the permutation. We define $\pi\mathbf{T}$ by

$$\pi T_{i_{\pi 1},i_{\pi 2},\ldots,i_{\pi q}} = T_{i_1,i_2,\ldots,i_q}.$$

As an example, consider the permutation

$$1,2,3,\ldots,q \to 3,1,8,7,2\ldots.$$

Then $\pi T_{i_{\pi 1},i_{\pi 2},\ldots,i_{\pi q}} = \pi T_{i_3,i_1,i_8,i_7,i_2,\ldots}$. By definition, this is equal to $T_{i_1,i_2,i_3}\ldots$, or alternatively $\pi T_{i_1,i_2,i_3,\ldots} = T_{i_2,i_5,i_1,\ldots}$.

As another example, let π be the permutation $i,j,k,l \to k,l,j,i$. Then

$$\pi T_{i,j,k,l} = T_{l,k,i,j}.$$

We define a totally symmetric tensor as follows: If $\pi T_{i_1,i_2,\ldots} = T_{i_1,i_2,\ldots}$ for all $q!\,\pi\mathbf{T}$, then $\mathbf{T}$ is said to be totally symmetric. In the last example above, this would for instance mean that $T_{l,k,i,j} = T_{i,j,k,l}$.

For any tensor $\mathbf{T}$ of order q we define the totally symmetric part $s\mathbf{T}$ of $\mathbf{T}$ as follows:

$$s\mathbf{T} = \frac{1}{q!}\sum \pi\mathbf{T}, \tag{2.5}$$

where the summation is over all $q!$ permutations.

EXAMPLE 4. For $q = 4$ the totally symmetric part of $\mathbf{T}$ becomes

$$S_{ijkl} = \frac{1}{24}(T_{ijkl} + T_{ijlk} + T_{ikjl} + T_{iklj} + T_{ilkj} + T_{iljk} + T_{jikl} + \cdots). \tag{2.6}$$

The expression for S_{ijkl} contains 24 addends. If $\mathbf{T}$ is totally symmetric, all the 24 tensor components in the parenthesis are equal.

Applying the normal elastic symmetry relations,

$$T_{ijkl} = T_{jikl} = T_{ijlk} = T_{klij},$$

(2.6) reduces to

$$S_{ijkl} = \frac{1}{3}(T_{ijkl} + T_{ikjl} + T_{iljk}). \tag{2.7}$$

Equation (2.7) coincides with the definition of the totally symmetric tensor in the article of Backus. Notice that Backus has a misprint in his definition.

EXAMPLE 5. Consider a tensor $\mathbf{T}$ of order 4. The polynomial $\mathbf{S}(\mathbf{r})$ generated by the totally symmetric tensor, by using equations (2.3) and (2.5) is

$$\mathbf{S}(\mathbf{r}) = x^4 T_{1111} + \frac{1}{4}x^3 y(T_{1112} + T_{1121} + T_{1211} + T_{2111}) + \cdots$$

$$+\frac{1}{4}x^3y(T_{1121}+T_{1112}+T_{1211}+T_{2111})$$
$$+\frac{1}{6}x^2y^2(T_{1122}+T_{2211}+T_{1212}+T_{1221}+T_{2121}+T_{2112})+\cdots$$
$$+z^4T_{3333}.$$

There are 81 parenthesis-expressions in this expansion for $\mathbf{S}(\mathbf{r})$. Before contraction each paranthesis contained 24 addends.

The monomial x^3y, for instance, occurs as often as the number of different combinations of the figures $1, 1, 1$ and 2, that is, four times. Each of the four terms in the parentheses occurs six times before contraction. The coefficient belonging to the term x^3y for each of the four places is

$$\frac{1}{4}(T_{1112}+T_{1121}+T_{1211}+T_{2111}).$$

Contracting all four paranthesis-expressions associated to x^3y gives the coefficient

$$T_{1112}+T_{1121}+T_{1211}+T_{2111}$$

which is the same as the coefficient belonging to x^3y in the contracted expression for $\mathbf{T}(\mathbf{r})$.

More generally, if there are m different combinations of the four dummy indices for a specific case, each of the m tensor components $(c_1, c_2, \ldots, c_m)$ occurs n times in the expression for the coefficient so that $mn = q!$. The monomial occurs m places in the polynomial $\mathbf{S}(\mathbf{r})$. After contracting terms with equal monomials, the coefficient is $(c_1 + c_2 + \cdots + c_m)$, which is also the coefficient belonging to this monomial in the expression for $\mathbf{T}(\mathbf{r})$; see (2.4).

We have thus illustrated the fact that the totally symmetric tensor $s\mathbf{T}$ generates the same polynomial as $\mathbf{T}$ itself.

Obviously different tensors can generate the same polynomial. However, only one totally symmetric tensor can generate a given polynomial. If one or more components change, then also the polynomial changes.

The coefficients in the totally symmetric tensor $\mathbf{S}$ can be obtained from the formula

$$S_{i_1,\ldots,i_q} = \frac{1}{q!}\partial_{i_1\ldots i_q}\mathbf{S}(\mathbf{r}), \tag{2.8}$$

where $\partial_{i_1\ldots i_q}$ denotes the qth-order partial derivative with respect to $r_{i_1}, \ldots, r_{i_q}$. As an example, let us calculate S_{1112} from the expression for $\mathbf{S}(\mathbf{r})$, where $N = 3$ and $q = 4$:

$$S_{1112} = \frac{1}{24}\frac{\partial}{\partial x^3\partial y}\mathbf{S}(\mathbf{r}) = \frac{1}{24}\times\frac{1}{4}(T_{1112}+T_{1121}+T_{1211}+T_{2111})\times 3\times 2\times 4$$
$$= \frac{1}{4}(T_{1112}+T_{1121}+T_{1211}+T_{2111}).$$

The same expression is obviously obtained for S_{1121}, S_{1211}, and S_{2111} By using the same definition trying to find the coefficient T_{1112} from $\mathbf{T}(\mathbf{r})$, we get

$$\frac{1}{24}(T_{1112} + T_{1121} + T_{1211} + T_{2111}) \times 3 \times 2$$

which is the same expression as above, but this is not generally the same as T_{1112}. To stress this result, (2.8) is not a formula for finding T_{ijkl}. Given a polynomial, there is no unique tensor corresponding to it. However, the components of the totally symmetric part of a tensor can be obtained from the polynomial $\mathbf{T}(\mathbf{r})$. It follows that there is a one-to-one correspondence between the homogeneous polynomials in P_N^q and the linear space S_N^q of all totally symmetric tensors of order q over V_N^q. The dimension of S_N^q and P_N^q are therefore equal. For $N = 3$ and $q = 4$, the dimension of S_N^q is 15. This means that a totally symmetric elastic tensor generally has 15 independent terms instead of 21. This is equal to the number of different monomials in the homogeneous polynomial generated by the tensor.

In summary, the number of components in a tensor is N^q; the number of different monomials in the generated homogeneous polynomial is equal to the dimension of the vectorspace of all homogeneous polynomials of degree q and dimension N; the number of independent components in the totally symmetric tensor is equal to the number of different monomials in the corresponding homogeneous polynomial; more than one tensor correspond to a specific homogeneous polynomial of degree q and dimension N; however, there is a unique totally symmetric tensor generating this polynomial.

2.5 Decomposition of the elasticity tensor into a totally symmetric part and an asymmetric part

Let us define an elastic tensor $\mathbf{E}$ as a tensor of order 4 and dimension 3, which satisfies

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}.$$

The linear space of all elastic tensors is denoted by E_3^4. The number of independent entries in an elastic tensor is 21, and the dimension of E_3^4 is therefore 21.

We will now decompose an arbitrary elastic tensor $\mathbf{E}$ into a totally symmetric tensor $s\mathbf{E}$ and an asymmetric part $\mathbf{A}$ ($\mathbf{A}$ still has the elastic symmetry). The asymmetric part is simply defined as $\mathbf{E} - s\mathbf{E}$. Equation (2.7) gives the expression for the totally symmetric part of an elastic tensor :

$$S_{ijkl} = \frac{1}{3}(E_{ijkl} + E_{ikjl} + E_{iljk}). \tag{2.9}$$

The asymmetric tensor is expressed as

$$A_{ijkl} = E_{ijkl} - S_{ijkl} = \frac{2}{3}E_{ijkl} - \frac{1}{3}E_{iklj} - \frac{1}{3}E_{iljk} \tag{2.10}$$

which has the elastic symmetry. The linear space of all asymmetric elastic tensors is denoted by A_3^4.

Any elastic tensor in E_3^4 can be expressed in the form

$$\mathbf{E} = \mathbf{S} + \mathbf{A},$$

where $\mathbf{S}$ is in S_3^4 and $\mathbf{A}$ is in A_3^4. Backus shows that E_3^4 is the direct sum of S_3^4 and A_3^4, where the direct sum of two vectorspaces A and B is defined as the set of all pairs x, y with x in A and y in B, and A and B are disjoint. Every vector in the direct sum can be written in the form $x + y$ in one and only one way. The dimension of the direct sum is the sum of the dimensions of the vectorspaces building the direct sum.

Since E_3^4 is the direct sum of S_3^4 and A_3^4, it follows that

$$\mathrm{Dim}\, E_3^4 = \mathrm{Dim}\, S_3^4 + \mathrm{Dim}\, A_3^4.$$

As shown in example 5, $\mathrm{Dim}\, E_3^4$ is 21 and $\mathrm{Dim}\, S_3^4$ is 15. It follows that $\mathrm{Dim}\, A_3^4$ is 6.

EXAMPLE 6. We shall now express all the components of S_{ijkl} in terms of E_{ijkl}. If we introduce the 2-subscript notation for the totally symmetric tensor and for the elastic tensor, we have by using (2.9)

$$s_{11} = S_{1111} = \frac{1}{3}(E_{1111} + E_{1111} + E_{1111}) = c_{11},$$

$$s_{12} = S_{1122} = \frac{1}{3}(E_{1122} + E_{1221} + E_{1212}) = \frac{1}{3}(c_{12} + 2c_{66}) = s_{66},$$

$$s_{13} = S_{1133} = \frac{1}{3}(E_{1133} + E_{1331} + E_{1313}) = \frac{1}{3}(c_{13} + 2c_{55}) = s_{55},$$

$$s_{14} = S_{1123} = \frac{1}{3}(E_{1123} + E_{1231} + E_{1312}) = \frac{1}{3}(c_{14} + 2c_{56}) = s_{56},$$

$$s_{15} = S_{1113} = \frac{1}{3}(E_{1113} + E_{1131} + E_{1311}) = c_{15},$$

$$s_{16} = S_{1112} = \frac{1}{3}(E_{1112} + E_{1121} + E_{1211}) = c_{16}.$$

Continuing in this way, we have

$$s_{22} = c_{22}, \quad s_{23} = \frac{1}{3}(c_{23} + 2c_{44}) = s_{44}, \quad s_{24} = c_{24},$$

$$s_{25} = \frac{1}{3}(c_{25} + 2c_{46}) = s_{46}, \quad s_{26} = c_{26}, \quad s_{33} = c_{33}, \quad s_{34} = c_{34},$$

$$s_{35} = c_{35}, \quad s_{36} = \frac{1}{3}(c_{36} + 2c_{45}) = s_{45}.$$

In matrix form, the totally symmetric tensor can be presented as

$$\begin{pmatrix} c_{11} & s_{66} & s_{55} & s_{56} & c_{15} & c_{16} \\ & c_{22} & s_{44} & c_{24} & s_{46} & c_{26} \\ & & c_{33} & c_{34} & c_{35} & s_{45} \\ & & & s_{44} & s_{45} & s_{46} \\ & & & & s_{55} & s_{56} \\ & & & & & s_{66} \end{pmatrix}$$

We notice that the nine terms s_{11}, s_{15}, s_{16}, s_{22}, s_{24}, s_{26}, s_{33}, s_{34}, and s_{35} are all equal to the corresponding elastic components. The remaining 12 components are pairwise equal, so that there are six more independent terms in the totally symmetric tensor, so there are 15 independent terms in total.

By using the formula for the asymmetric tensor, we would find that the nine terms with indices (11), (15), (16), (22), (24), (26), (33), (34), and (35) are all equal to zero, as they should be. There are six independent terms.

In matrix form, the asymmetric tensor can be presented as

$$\begin{pmatrix} 0 & -2a_{66} & -2a_{55} & -2a_{56} & 0 & 0 \\ & 0 & -2a_{44} & 0 & -2a_{46} & 0 \\ & & 0 & 0 & 0 & -2a_{45} \\ & & & a_{44} & a_{45} & a_{46} \\ & & & & a_{55} & a_{56} \\ & & & & & a_{66} \end{pmatrix} \tag{2.11}$$

Cowin **(2)** defines a totally symmetric tensor as

$$S^C_{ijkl} = \frac{1}{2}(E_{ijkl} + E_{ikjl}). \tag{2.12}$$

We shall show that this tensor is not totally symmetric. According to Cowin we have

$$S^C_{ijlk} = \frac{1}{2}(E_{ijlk} + E_{iljk}) = \frac{1}{2}(E_{ijkl} + E_{iljk})$$

which is in general different from S^C_{ijkl}.

As an example, let us find S^C_{1231} and S^C_{1213} from (2.12):

$$S^C_{1231} = \frac{1}{2}(E_{1231} + E_{1321}) = \frac{1}{2}(c_{56} + c_{56}) = c_{56},$$

$$S^C_{1213} = \frac{1}{2}(E_{1213} + E_{1123}) = \frac{1}{2}(c_{56} + c_{14}).$$

Since S^C_{1231} and S^C_{1213} are different, (2.12) does not define a totally symmetric tensor. See also Cowin **(6)** where the totally symmetric part is defined as in (2.9).

Is it possible to describe the asymmetric part of the elastic tensor in terms of totally symmetric tensors? Let as before S^q_N denote the linear space of all totally symmetric tensors, and let A_3^4 denote the linear space of all asymmetric elastic tensors.

According to Backus there exists a one-to-one mapping such that to each A there corresponds a totally symmetric tensor of order 2, and dimension 3. In the following we shall show the explicit expression for this mapping.

Let $\phi(S_3^2)$ denote the linear space of all asymmetric tensors $\mathbf{A}$ in A_3^4 for which there is a totally symmetric tensor $\mathbf{t}$ in S_3^2 such that $\mathbf{A} = \phi(\mathbf{t})$. Notice that $\mathrm{Dim}\,\phi(S_3^2) = \mathrm{Dim}\,S_3^2$, because of the one-to-one mapping between the two spaces.

The order of the tensors in the two vector spaces are 4 and 2 respectively. In $\phi(S_3^2)$ the tensors are asymmetric, and in S_3^2 the tensors are totally symmetric.

Any elastic tensor can then be expressed as $\mathbf{E} = \mathbf{S} + \mathbf{A}$ where $\mathbf{A} = \phi(\mathbf{t})$. The $\mathbf{S}$ and $\mathbf{t}$ are unique totally symmetric tensors of order 4 and 2 respectively. The one-to-one mapping $\phi(\mathbf{t})$ is given by

$$A_{ijkl} = \delta_{ij}t_{kl} + \delta_{kl}t_{ij} - \frac{1}{2}\delta_{ik}t_{jl} - \frac{1}{2}\delta_{jl}t_{ik} - \frac{1}{2}\delta_{il}t_{jk} - \frac{1}{2}\delta_{jk}t_{il}. \tag{2.13}$$

This equation can also be solved with respect to t_{ij}:

$$t_{ij} = A_{ijpp} - \frac{\delta_{ij}}{4}A_{rrpp} \tag{2.14}$$

Let us consider some examples of tensors defined so far. Figures 2.1, 2.2 and 2.3 show the elasticity tensor, the asymmetric tensor, and the second-order totally symmetric tensor associated with the asymmetric tensor for an orthorhombic, a monoclinic and a triclinic medim. The asymmetric tensor is calculated from (2.10).

The figures shows that (2.11) is satisfied with an uncertainty of 1 in the last digit. The totally symmetric part is the difference between the elasticity tensor and the asymmetric part. The figures shows that only in the triclinic and the monoclinic case do second-order totally symmetric tensors have off-diagonal components different from zero. For symmetry systems of orthorhombic and higher symmetry, the off-diagonal components are equal to zero.

Let us consider this second-order tensor more carefully. According to (2.14), the off-diagonal components of the second-order tensor are expressed as

$$t_{12} = A_{1211} + A_{1222} + A_{1233} = a_{16} + a_{26} + a_{36},$$

$$t_{13} = A_{1311} + A_{1322} + A_{1333} = a_{15} + a_{25} + a_{35},$$

$$t_{23} = A_{2311} + A_{2322} + A_{2333} = a_{14} + a_{24} + a_{34}.$$

(2.11) shows that only a_{14}, a_{25} and a_{36} of the nine components of the asymmetric tensor above can be different from zero. Those three components are obviously equal to zero when the corresponding elasticity components c_{14}, c_{25} and c_{36} are equal to zero. But c_{14}, c_{25} and c_{36} are all equal to zero for all crystal systems apart from

$$
\text{(i)} \quad \begin{pmatrix} 3.150 & 1.950 & 1.850 & 0 & 0 & 0 \\ & 2.750 & -1.350 & 0 & 0 & 0 \\ & & 6.650 & 0 & 0 & 0 \\ & & & 2.550 & 0 & 0 \\ & & & & 2.600 & 0 \\ & & & & & 2.450 \end{pmatrix}
$$

$$
\text{(ii)} \quad \begin{pmatrix} 0 & -0.333 & -0.500 & 0 & 0 & 0 \\ & 0 & -2.600 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 1.300 & 0 & 0 \\ & & & & 0.250 & 0 \\ & & & & & 0.167 \end{pmatrix}
$$

$$
\text{(iii)} \quad \begin{pmatrix} 0.883 & 0 & 0 \\ & -1.217 & 0 \\ & & -1.383 \end{pmatrix}
$$

Figure 2.1: Orthorhombic tensor, matrix form. (i) The elasticity tensor, (ii) the associated asymmetric tensor and (iii) the related second-order tensor. The second-order tensor is diagonal.

$$\text{(i)} \quad \begin{pmatrix} 3.150 & 1.950 & 1.850 & 0 & 0 & 1.100 \\ & 2.750 & -1.350 & 0 & 0 & 1.000 \\ & & 6.650 & 0 & 0 & 2.000 \\ & & & 2.550 & 0.850 & 0 \\ & & & & 2.600 & 0 \\ & & & & & 2.450 \end{pmatrix}$$

$$\text{(ii)} \quad \begin{pmatrix} 0 & -0.333 & -0.500 & 0 & 0 & 0 \\ & 0 & -2.600 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0.767 \\ & & & 1.300 & -0.383 & 0 \\ & & & & 0.250 & 0 \\ & & & & & 0.167 \end{pmatrix}$$

$$\text{(iii)} \quad \begin{pmatrix} 0.883 & 0.767 & 0 \\ & -1.217 & 0 \\ & & -1.383 \end{pmatrix}$$

Figure 2.2: Monoclinic tensor, matrix form. (i) The elasticity tensor, (ii) the associated asymmetric tensor and (iii) the related second-order tensor. The second-order tensor is not diagonal.

$$
\text{(i)} \quad \begin{pmatrix}
3.150 & 1.950 & 1.850 & 2.000 & 2.000 & 1.100 \\
 & 2.750 & -1.350 & 1.100 & 1.200 & 1.000 \\
 & & 6.650 & 1.000 & 1.300 & 2.000 \\
 & & & 2.550 & 1.000 & 1.000 \\
 & & & & 2.600 & 1.350 \\
 & & & & & 2.450
\end{pmatrix}
$$

$$
\text{(ii)} \quad \begin{pmatrix}
0 & -0.333 & -0.500 & 0.433 & 0 & 0 \\
 & 0 & -2.600 & 0 & 0.133 & 0 \\
 & & 0 & 0 & 0 & 0.667 \\
 & & & 1.300 & -0.333 & -0.067 \\
 & & & & 0.250 & -0.217 \\
 & & & & & 0.167
\end{pmatrix}
$$

$$
\text{(iii)} \quad \begin{pmatrix}
0.883 & 0.667 & 0.133 \\
 & -1.217 & 0.433 \\
 & & -1.383
\end{pmatrix}
$$

Figure 2.3: Triclinic tensor, matrix form. (i) The elasticity tensor, (ii) the associated asymmetric tensor and (iii) the related second-order tensor. The second-order tensor is not diagonal.

the triclinic, monoclinic and the trigonal cases, see Helbig (**7**) or Musgrave (**4**). By expressing t_{12}, t_{13} and t_{23} by means of elastic constants, we have

$$t_{12} = a_{36} = A_{1233} = \frac{2}{3}E_{1233} - \frac{1}{3}E_{1323} - \frac{1}{3}E_{1323} = \frac{2}{3}(c_{36} - c_{45}),$$

and similarly

$$t_{13} = \frac{2}{3}(c_{25} - c_{46}), \qquad t_{23} = \frac{2}{3}(c_{14} - c_{56}).$$

By using the relations between elastic constants for monoclinic and trigonal symmetry, we find that there are off-diagonal terms in the second-order totally symmetric tensor only in the monoclinic case in addition to the triclinic case.

The tensors above are related to a coordinate system with the 3-axis as the symmetry axis. If for instance the 2-axis is used as symmetry axis, the elasticity tensor for monoclinic media look different from the tensor in Fig. 2.2. (see (**3**)). However, for a symmetric medium, there is a symmetry coordinate system where the second-order symmetric tensor related to the asymmetric part of the elasticity tensor is diagonal. The coordinate axes are the eigenvectors of this second-order tensor.

2.6 Determination of a symmetry coordinate system

Fig. 2.4 shows a monoclinic system in its symmetry coordinate system. The second-order tensor is not diagonal. With the eigenvectors of the second-order tensor as the new coordinate system, this tensor becomes diagonal. In the new coordinate system, the elasticity tensor is still monoclinic, but now with the 2-axis as symmetry axis. By rotation of the coordinate system by 90 degrees around the 1-axis, the 3-axis is again the symmetry axes.

For the monoclinic medium in Fig. 2.5 the elasticity tensor is not recorded in a symmetry coordinate system (21 elastic constants). The tensor is produced by starting with the monoclinic tensor in Fig. 2.4, and then rotated arbitrary fixed angles around each of the three axes. All the elements in the tensor are different from zero. The second-order symmetric tensor has all elements different from zero. The eigenvalues and eigenvectors for the second-order tensor are calculated. When the eigenvectors are used as a new coordinate system, the elasticity tensor shows that the medium is monoclinic. The transformed tensor is equal to the transformed tensor in Fig. 2.4. If the diagonalization process is done with the transformed tensor as original tensor, the second-order tensor is diagonal as it should be, and the eigenvectors in this case are just the coordinate axes, and the transformed tensor is equal to the original tensor. Notice that the transformed tensor is different from the monoclinic tensor in Figs. 2.2 and 2.4 where the 3-axis is the symmetry axis. In Fig. 2.4 the transformed tensors are given in a symmetry system with the 2-axis as symmetry axis.

$$
\text{(i)} \quad \begin{pmatrix}
3.150 & 1.950 & 1.850 & 0.000 & 0.000 & 1.100 \\
 & 2.750 & -1.350 & 0.000 & 0.000 & 1.000 \\
 & & 6.650 & 0.000 & 0.000 & 2.000 \\
 & & & 2.550 & 0.850 & 0.000 \\
 & & & & 2.600 & 0.000 \\
 & & & & & 2.450
\end{pmatrix}
$$

$$
\text{(ii)} \quad \begin{pmatrix}
0.883 & 0.767 & 0 \\
 & -1.217 & 0 \\
 & & -1.383
\end{pmatrix}
$$

$$
\text{(iii)} \quad \begin{pmatrix} -1.4667 & -1.3833 & 1.1334 \end{pmatrix}
$$

$$
\text{(iv)} \quad \begin{pmatrix}
-0.3101 & 0.0000 & -0.9507 \\
0.9507 & 0.0000 & -0.3101 \\
0.0000 & 1.0000 & 0.0000
\end{pmatrix}
$$

$$
\text{(v)} \quad \begin{pmatrix}
2.276 & -2.222 & 1.224 & 0.000 & 0.155 & 0.000 \\
 & 6.650 & 2.722 & 0.000 & -0.672 & 0.000 \\
 & & 5.076 & 0.000 & -1.733 & 0.000 \\
 & & & 3.096 & 0.000 & -0.672 \\
 & & & & 1.724 & 0.000 \\
 & & & & & 2.054
\end{pmatrix}
$$

Figure 2.4: (i) Monoclinic tensor referred to symmetry coordinate system. The 3-axis is the symmetry axis. (ii) The tensor is transformed to symmetry coordinate system by diagonalization of the second-order tensor related to the asymmetric tensor. The 2-axis is now the symmetry axis. (iii) Eigenvalues and (iv) eigenvectors of the matrix (ii). (v) The elasticity matrix after transformation.

$$
\text{(i)} \quad \begin{pmatrix}
3.839 & 0.091 & 0.966 & -1.144 & 1.719 & -0.508 \\
 & 7.700 & 0.213 & 0.518 & 1.217 & -0.800 \\
 & & 3.370 & 0.384 & 1.015 & -0.139 \\
 & & & 1.244 & 0.810 & 0.139 \\
 & & & & 2.939 & 0.435 \\
 & & & & & 2.238
\end{pmatrix}
$$

$$
\text{(ii)} \quad \begin{pmatrix}
-1.030 & -0.632 & 0.718 \\
 & -0.402 & -1.052 \\
 & & -0.285
\end{pmatrix}
$$

$$
\text{(iii)} \quad \begin{pmatrix} -1.4667 & -1.3833 & 1.1334 \end{pmatrix}
$$

$$
\text{(iv)} \quad \begin{pmatrix}
-0.8332 & 0.3770 & 0.4045 \\
0.0494 & 0.7794 & -0.6246 \\
0.5507 & 0.5004 & 0.6681
\end{pmatrix}
$$

$$
\text{(v)} \quad \begin{pmatrix}
2.276 & -2.222 & 1.224 & 0.000 & 0.155 & 0.000 \\
 & 6.650 & 2.722 & 0.000 & -0.672 & 0.000 \\
 & & 5.076 & 0.000 & -1.733 & 0.000 \\
 & & & 3.096 & 0.000 & -0.672 \\
 & & & & 1.724 & 0.000 \\
 & & & & & 2.054
\end{pmatrix}
$$

Figure 2.5: Monoclinic tensor, 21 elastic constants. Transformed to symmetry coordinate system by diagonalization as in Fig. 2.4.

For a monoclinic tensor it is always possible to remove c_{36} or c_{45} by a rotation around the symmetry axis (3-axis). Thus the tensors in Fig. 2.4 have 12 elastic constants after such a rotation.

By producing different tensors with the original monoclinic tensor as starting point, the transformed tensor in the diagonalization process is always the same.

The method of diagonalization is applied to all different symmetry systems. For cubic symmetry, the second-order tensor related to the asymmetric tensor is diagonal in all coordinate systems. Thus it is not possible to find a symmetry coordinate system by this method for cubic symmetry. However, use of Maxwell multipoles will identify the four diagonals. The symmetry coordinate system is then known. See also the discussion in section 2.13 on Maxwell multipoles where cubic symmetry is used as an example.

In summary, it has been shown that the second-order tensor related to the asymmetric elastic tensor is diagonal when the elastic tensor is recorded in a symmetry coordinate system. Further, that by diagonalizing the second-order symmetric tensor related to the asymmetric tensor, the eigenvectors form a symmetry coordinate system for the medium. For cubic symmetry, Maxwell multipoles will identify the symmetry coordinate system.

2.7 Harmonic representations

A function $f(r)$ in V_N is said to be harmonic if $\Delta f(r) = 0$, where Δ is the Laplace operator. The harmonic polynomials $P(r)$ in P_N^q are called solid spherical harmonics of degree q. They constitute a linear subspace H_N^q of P_N^q.

The following equality is valid (see Backus) (**1**)):

$$\Delta[r^n H^{(q)}(r)] = n(2q + n + N - 2)r^{n-2}H^{(q)}(r). \tag{2.15}$$

It follows from Courant and Hilbert (**8**) that if $P^{(q)}(r)$ is any homogeneous polynomial of degree q and dimension N, then there are unique harmonic polynomials $H^{(q)}(r), H^{(q-2)}(r), \dots$ of dimension N and degree q, $q-2$, $\dots$ such that

$$P^{(q)}(r) = H^{(q)}(r) + r^2 H^{(q-2)}(r). + r^4 H^{(q-4)}(r) + \cdots. \tag{2.16}$$

For $q = 4$ we have

$$P^{(4)}(r) = H^{(4)}(r) + r^2 H^{(2)}(r) + r^4 H^{(0)}(r).$$

According to Backus, a totally symmetric tensor $\mathbf{S}$ generates a harmonic polynomial if and only if the tensor is totally traceless. This means that $\Delta\mathbf{S}(\mathbf{r}) = 0$ if and only if $\mathrm{tr}_{ij}\mathbf{S} = 0$ for any pair of distinct indices i and j. We shall show this in the case when $q = 4$ and $N = 3$. Let $\mathbf{H}(\mathbf{r})$ be the harmonic polynomial generated by a totally symmetric tensor $\mathbf{H}$. Since $\mathbf{H}(\mathbf{r})$ is harmonic, $\Delta\mathbf{H}(\mathbf{r}) = 0$. From example 2 it is easily seen that $\mathbf{H}(\mathbf{r})$ can be written as

$$\mathbf{H}(\mathbf{r}) = x^4 H_{1111} + 4x^3 y H_{1112} + 4x^3 z H_{1113} + 6x^2 y^2 H_{1122}$$

$$6x^2 z^2 H_{1133} + 12x^2 yz H_{1123} + \cdots$$

By applying the Laplace operator we have

$$\Delta\mathbf{H}(\mathbf{r}) = 4 \times 3x^2 H_{1111} + 4 \times 3 \times 2xy H_{1112} + 4 \times 3 \times 2xz H_{1113}$$

$$+6 \times 2y^2 H_{1122} + \cdots + 6 \times 2x^2 H_{1122} + 4 \times 3 \times 2xy H_{2212}$$

$$12 \times 2xz H_{2213} + \cdots + 6 \times 2x^2 H_{1133} + 12 \times 2xy H_{3312} \cdots$$

$$+4 \times 3z^2 H_{3333} = 0.$$

Contracting and rearranging gives

$$x^2(H_{1111} + H_{2211} + H_{3311}) + 2xy(H_{1112} H_{2212} + H_{3312})$$

$$2xz(H_{1113} + H_{2213} + H_{3313}) + y^2(H_{1122} + H_{2222} + H_{3322})$$

$$+2yz(H_{1123} + H_{2223} + H_{3323}) + z^2(H_{1133} + H_{2233} + H_{3333}) = 0.$$

The coefficients in this polynomial are the components of the tensor $H_{jji_3i_4} = \operatorname{tr}_{12}\mathbf{H}$ if $\mathbf{H}$ is totally symmetric. The polynomial is equal to zero for all values of the coordinates. Generally, if a polynomial is equal to zero for all values of the coordinates, then all the coefficients are equal to zero. The coefficients in the polynomial above must therefore vanish. Since the coefficients in this specific polynomial are equal to the components of the tensor $H_{jji_3i_4}$, all the components in this tensor must vanish.

Since $\mathbf{H}$ is totally symmetric, $\operatorname{tr}_{ij}\mathbf{H} = 0$ for any pair of distinct indices i and j. This illustrates the fact that $\operatorname{tr}_{ij}\mathbf{H} = 0$ if and only if $\Delta\mathbf{H}(\mathbf{r}) = 0$ for a totally symmetric tensor. A harmonic tensor $\mathbf{H}$ is defined to be a totally symmetric traceless tensor.

Corresponding to (2.16), any totally symmetric tensor $\mathbf{S}$ has a decomposition into harmonic tensors $\mathbf{H}^{(q)}$, $\mathbf{H}^{(q-2)}$, $\cdots$ as follows:

$$\mathbf{S} = \mathbf{H}^{(q)} + s(\mathbf{I}\mathbf{H}^{(q-2)}) + s(\mathbf{I}\mathbf{I}H^{(q-4)}) + \cdots, \tag{2.17}$$

where s denotes the totally symmetric part.

Let us verify equation (2.17) for the case when $q = 4$ and $N = 3$. We shall start with a comment on tensor products. Let S_{ij} and T_{kl} be two totally symmetric tensors. Then $A_{ijkl} = S_{ij}T_{kl}$ is the product. Now $A_{ikjl} = S_{ik}T_{jl}$ is not generally equal to A_{ijkl}. This shows that assuming two tensors to be totally symmetric does not imply the tensor product to be totally symmetric. For second-order tensors, total symmetry is the same as symmetry.

In (2.16), $r^2 = x^2 + y^2 + z^2$ is the homogeneous polynomial generated by the identity tensor $\mathbf{I} = \delta_{ij}$ and $r^4 = x^4 + y^4 + z^4 + 2x^2y^2 + 2x^2z^2 + 2y^2z^2$ is generated by $\mathbf{II} = \delta_{ij}\delta_{kl}$.

To each homogeneous polynomial $P(r)$ corresponds a unique totally symmetric tensor $\mathbf{S}$. To the harmonic polynomials $H^{(4)}(r), H^{(2)}(r)$, and $H^{(0)}(r)$ correspond the unique harmonic tensors $\mathbf{H}^{(4)}, \mathbf{H}^{(2)}$, and $H^{(0)})$ respectively.

To $r^2H^{(2)}(r)$ and $r^4H^{(0)}(r)$ correspond $s[\mathbf{IH}^{(2)}]$ and $s[\mathbf{II}H^{(0)}]$ respectively, where s denotes the totally symmetric part. The $\mathbf{IH}^{(2)}$ and $\mathbf{IIH}^{(0)}$ are tensorproducts. Notice that $\mathbf{IH}^{(2)}$ and $\mathbf{II}$ are not totally symmetric although $\mathbf{I}$ and $\mathbf{H}^{(2)}$ are totally symmetric. We conclude, then, by (2.16), that a totally symmetric tensor $\mathbf{S}$ can be decomposed into totally symmetric tensors as

$$\mathbf{S} = \mathbf{H}^{(4)} + s(\mathbf{IH}^{(2)}) + s(\mathbf{IIH}^{(0)}). \tag{2.18}$$

2.8 Harmonic decomposition of the elasticity tensor

We shall now express $\mathbf{E}$ in terms of the components of the harmonic tensors. From (2.18) we have

$$\mathbf{S} = \mathbf{H}^{(4)} + 6s(\mathbf{IH}^{(2)}) + 3s(\mathbf{II}H^{(0)}). \tag{2.19}$$

where $\mathbf{H}^{(2)}$ and $\mathbf{H}^{(0)}$ now are constant multiples of the harmonics in (2.18).

Since $\mathbf{t}$ is a second-order symmetric tensor, $\mathbf{t}$ can be decomposed as

$$\mathbf{t} = \mathbf{h}^{(2)} + \frac{1}{2}\mathbf{Ih}^{(0)}. \tag{2.20}$$

The factors 6, 3, and $\frac{1}{2}$ appear in (2.19) and (2.20) to obtain simple expressions in the further calculations. We have

$$\phi(\mathbf{t}) = \phi(\mathbf{h}^{(2)} + \frac{1}{2}\mathbf{Ih}^{(0)}) = \phi(\mathbf{h}^{(2)}) + \frac{1}{2}\phi(\mathbf{Ih}^{(0)}).$$

since ϕ is linear. The decomposition of $\mathbf{E}$ can then be written as

$$\mathbf{E} = \mathbf{H}^{(4)} + 6s(\mathbf{IH}^{(2)}) + 3s(\mathbf{IIH}^{(0)}) + \phi(\mathbf{h}^{(2)}) + \frac{1}{2}\phi(\mathbf{Ih}^{(0)}).$$

Notice that all five harmonic tensors are uniquely determined by $\mathbf{E}$. We shall start by finding $s(\delta_{ij}H_{kl})$. From four elements, i, j, k and l, there are six possibilities of choosing groups of 2 : (ij), (kl), (ik), (jl), (il), and (jk). The totally symmetric part of $\delta_{ij}H_{kl}$ is then

$$s(\delta_{ij}H_{kl}) = \frac{1}{6}[\delta_{ij}H_{kl} + \delta_{kl}H_{ij} + \delta_{ik}H_{jl} + \delta_{jl}H_{ik} + \delta_{il}H_{jk} + \delta_{jk}H_{il}].$$

Similarly, the totally symmetric part of $\delta_{ij}\delta_{kl}$ is

$$s(\delta_{ij}\delta_{kl}) = \frac{1}{3}[\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}].$$

Substitution in (2.19) gives

$$\begin{aligned} S_{ijkl} = H_{ijkl} + [\delta_{ij}H_{kl} + \delta_{kl}H_{ij} + \delta_{ik}H_{jl} + \delta_{jl}H_{ik} + \delta_{il}H_{jk} + \delta_{jk}H_{il}] \\ +H[\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}]. \end{aligned} \tag{2.21}$$

Substitution of (2.20) in (2.13) gives

$$\begin{aligned} A_{ijkl} &= \delta_{ij}(h_{kl} + \frac{1}{2}h\delta_{kl}) + \delta_{kl}(h_{ij} + \frac{1}{2}h\delta_{ij}) - \frac{1}{2}\delta_{ik}(h_{jl} + \frac{1}{2}h\delta_{jl}) \\ &-\frac{1}{2}\delta_{jl}(h_{ik} + \frac{1}{2}h\delta_{ik}) - \frac{1}{2}\delta_{il}(h_{jk} + \frac{1}{2}h\delta_{jk}) - \frac{1}{2}\delta_{jk}(h_{il} + \frac{1}{2}h\delta_{il}) \\ &= \delta_{ij}h_{kl} + \delta_{kl}h_{ij} - \frac{1}{2}\delta_{ik}h_{jl} - \frac{1}{2}\delta_{jl}h_{ik} - \frac{1}{2}\delta_{il}h_{jk} - \frac{1}{2}\delta_{jk}h_{il} \\ &\quad +h[\delta_{ij}\delta_{kl} - \frac{1}{2}\delta_{ik}\delta_{jl} - \frac{1}{2}\delta_{il}\delta_{jk}]. \end{aligned} \tag{2.22}$$

Adding (2.21) and (2.22) gives

$$\begin{aligned} E_{ijkl} = H_{ijkl} + [\delta_{ij}H_{kl} + \delta_{kl}H_{ij} + \delta_{ik}H_{jl} + \delta_{jl}H_{ik} + \delta_{il}H_{jk} + \delta_{jk}H_{il}] \\ +H[\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] \\ +\delta_{ij}h_{kl} + \delta_{kl}h_{ij} - \frac{1}{2}\delta_{ik}h_{jl} - \frac{1}{2}\delta_{jl}h_{ik} - \frac{1}{2}\delta_{il}h_{jk} - \frac{1}{2}\delta_{jk}h_{il} \\ +h[\delta_{ij}\delta_{kl} - \frac{1}{2}\delta_{ik}\delta_{jl} - \frac{1}{2}\delta_{il}\delta_{jk}]. \end{aligned} \tag{2.23}$$

2.9 Dilatational modulus tensor and Voigt tensor

The dilatational modulus tensor and the Voigt tensor are defined by

$$C_{ij} = E_{ijkk} \quad \text{and} \quad V_{ij} = E_{ikjk}$$

respectively, where $\mathbf{E}$ is the elasticity tensor. See Cowin **(2)** for a further discussion. The traces of these tensors are

$$\operatorname{tr}\mathbf{C} = C_{jj} = E_{jjkk} \quad \text{and} \quad \operatorname{tr}\mathbf{V} = V_{jj} = E_{jkjk}.$$

The deviatoric part of a tensor $\mathbf{T}$ is defined as

$$\hat{\mathbf{T}} = \mathbf{T} - \frac{1}{3}\mathbf{I}\operatorname{tr}\mathbf{T}.$$

The expression for the deviatoric part of C_{ij} and V_{ij} in terms of $\mathbf{E}$ are then

$$\hat{C}_{ij} = C_{ij} - \frac{1}{3}\delta_{ij}\operatorname{tr}C_{ij} = E_{ijkk} - \frac{1}{3}\delta_{ij}E_{ppkk} \quad \text{and} \quad \hat{V}_{ij} = E_{ikjk} - \frac{1}{3}\delta_{ij}E_{pkpk}.$$

2.10 Inversion of the harmonic decomposition

Assume now that the elasticity tensor E_{ijkl} is given. We shall express each of the harmonic tensors in terms of the the elasticity tensor. Contracting with respect to the last two indices in S_{ijkl} in (2.21) gives

$$S_{ijkk} = H_{ijkk} + [\delta_{ij}H_{kk} + \delta_{kk}H_{ij} + \delta_{ik}H_{jk} + \delta_{jk}H_{ik} + \delta_{ik}H_{jk} + \delta_{jk}H_{ik}]$$
$$+H[\delta_{ij}\delta_{kk} + \delta_{ik}\delta_{jk} + \delta_{ik}\delta_{jk}].$$
$$= H_{ijkk} + [\delta_{ij}H_{kk} + 3H_{ij} + H_{ij} + H_{ij} + H_{ij} + H_{ij} + H[3\delta_{ij} + \delta_{ij} + \delta_{ij}].$$

Since the harmonic tensors are traceless, $H_{ijkk} = 0$ and $\delta_{ij}H_{kk} = 0$. Hence

$$S_{ijkk} = 7H_{ij} + 5H\delta_{ij}. \tag{2.24}$$

Contracting gives

$$S_{jjkk} = 15H; \tag{2.25}$$

$H_{jj} = 0$ since H_{ij} is a harmonic tensor, and $\delta_{jj} = 3$. Backus has a misprint in the formula (2.25). From (2.9) we have

$$S_{ijkk} = \frac{1}{3}(E_{ijkk} + E_{ikkj} + E_{ikjk}) = \frac{1}{3}(E_{ijkk} + 2E_{ikjk}) \tag{2.26}$$

Equations (2.25) and (2.26) now give H in terms of $\mathbf{E}$:

$$H = \frac{1}{15}S_{jjkk} = \frac{1}{45}(E_{jjkk} + 2E_{jkjk}).$$

By using (2.24) and (2.25) we get

$$H_{ij} = \frac{1}{7}S_{ijkk} - \frac{5}{7}H\delta_{ij} = \frac{1}{7}[S_{ijkk} - \frac{1}{3}S_{ppkk}\delta_{ij}].$$

The above equation and (2.26) then give H_{ij} in terms of $\mathbf{E}$:

$$H_{ij} = \frac{1}{21}[E_{ijkk} - \frac{1}{3}E_{ppkk}\delta_{ij} + 2(E_{ikjk} - \frac{1}{3}E_{pkpk}\delta_{ij})].$$

By introducing the dilatational modulus, Voigt tensor, $\mathrm{tr}\,\mathbf{C}$ and $\mathrm{tr}\,\mathbf{V}$, H and H_{ij} can be expressed as follows:

$$H = \frac{1}{45}(\mathrm{tr}\,\mathbf{C} + 2\mathrm{tr}\,\mathbf{V}), \tag{2.27}$$

$$H_{ij} = \frac{1}{21}(\hat{C}_{ij} + 2\hat{V}_{ij}). \tag{2.28}$$

To get a simple expression for H_{ijkl}, define

$$Q_{ij} = \frac{(E_{ijmm} + 2E_{imjm})}{21} = \frac{(C_{ij} + 2V_{ij})}{21}.$$

Then $H = \frac{7}{15}Q_{jj}$ and $H_{ij} = Q_{ij} - \frac{1}{3}\delta_{ij}Q_{kk}$. Substituting $S_{ijkl} = \frac{1}{3}(E_{ijkl} + E_{iklj} + E_{iljk})$ and the expressions for H_{ij} and H into (2.21) gives

$$H_{ijkl} = \frac{1}{3}(E_{ijkl} + E_{jklj} + E_{iljk}) - Q_{ij}\delta_{kl} - Q_{kl}\delta_{ij} - Q_{ik}\delta_{jl} - Q_{jl}\delta_{ik} - Q_{il}\delta_{jk}$$
$$-Q_{jk}\delta_{il} + \frac{1}{5}Q_{mm}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{2.29}$$

By using (2.27) and (2.28) in the substitution above, we would have a more complicated expression for H_{ijkl}. However, it is obviously possible to express H_{ijkl} in terms of $\hat{\mathbf{C}}, \hat{\mathbf{V}}, \operatorname{tr}\mathbf{C}$, and $\operatorname{tr}\mathbf{V}$.

To find the expressions for h and h_{ij}, use equations (2.14), (2.20), and (2.10). We then have

$$h = \frac{1}{9}(E_{mmpp} - E_{mpmp}), \tag{2.30}$$

$$h_{ij} = \frac{2}{3}(E_{ijpp} - E_{ipjp}) - \frac{2}{9}\delta_{ij}(E_{rrpp} - E_{rprp}). \tag{2.31}$$

These two expressions differ from the expressions in the article of Backus by a factor of 2. However, calculations later in this article support that (2.30) and (2.31) are correct. In terms of $\hat{\mathbf{C}}, \hat{\mathbf{V}}, \operatorname{tr}\mathbf{C}$, and $\operatorname{tr}\mathbf{V}$, (2.30) and (2.31) are expressed as

$$h = \frac{1}{9}(\operatorname{tr}\mathbf{C} - \operatorname{tr}\mathbf{V}), \tag{2.32}$$

$$h_{ij} = \frac{2}{3}(\hat{C}_{ij} - \hat{V}_{ij}). \tag{2.33}$$

2.11 Decomposition and inversion according to Cowin

In Cowin (**2**), the elastic tensor $\mathbf{E}$ is decomposed as

$$E_{ijkl} = a\delta_{ij}\delta_{kl} + b[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] + \delta_{ij}\hat{A}_{kl} + \delta_{kl}\hat{A}_{ij}$$
$$+[\delta_{ik}\hat{B}_{jl} + \delta_{jl}\hat{B}_{ik} + \delta_{il}\hat{B}_{jk} + \delta_{jk}\hat{B}_{il}] + Z_{ijkl}, \tag{2.34}$$

where a and b are scalars, $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ are two second-order harmonic tensors, and $\mathbf{Z}$ is a fourth-order harmonic tensor.

From (2.34) we find $C_{ij}, V_{ij}, \operatorname{tr}\mathbf{C}$, and $\operatorname{tr}\mathbf{V}$, in terms of $\hat{\mathbf{A}}, \hat{\mathbf{B}}, a$, and b, where we use the fact that $\operatorname{tr}\hat{\mathbf{A}} = \operatorname{tr}\hat{\mathbf{B}} = \operatorname{tr}\hat{\mathbf{Z}} = 0$. Then $\hat{\mathbf{A}}, \hat{\mathbf{B}}, a$, and b can be uniquely expressed in terms of $\hat{\mathbf{C}}, \hat{\mathbf{V}}, \operatorname{tr}\mathbf{C}$, and $\operatorname{tr}\mathbf{V}$ as follows:

$$\hat{A}_{ij} = \frac{1}{7}(5\hat{C}_{ij} - 4\hat{V}_{ij}), \qquad \hat{B}_{ij} = \frac{1}{7}(3\hat{V}_{ij} - 2\hat{C}_{ij}), \tag{2.35}$$

$$a = \frac{1}{15}(2\operatorname{tr}\mathbf{C} - \operatorname{tr}\mathbf{V}), \qquad b = \frac{1}{30}(3\operatorname{tr}\mathbf{V} - \operatorname{tr}\mathbf{C}). \tag{2.36}$$

2.12 Comparing the theories of Backus and Cowin

Comparing Cowin's harmonic tensors in (2.35) and (2.36) with the expression for the corresponding tensors of Backus, none of the expressions are the same in the two sets of harmonic tensors. From Backus' decomposition we have, for example,

$$H_{12} = \frac{1}{21}(3c_{16} + 3c_{26} + c_{36} + c_{45}), \quad h_{12} = \frac{2}{3}(c_{36} - c_{45}).$$

The second-order harmonic tensors from Cowin's decomposition give

$$\hat{A}_{12} = \frac{1}{7}(c_{16} + c_{26} + 5c_{36} - 4c_{45}), \quad \hat{B}_{12} = \frac{1}{7}(c_{16} + c_{26} - 2c_{36} + 3c_{45}).$$

Neither of $\hat{A}_{12}$ and $\hat{B}_{12}$ is equal to H_{12} or h_{12}. However, it can be shown that there is a linear relationship between the two sets of tensors. Every elastic tensor can be expressed as a sum of the totally symmetric part and the asyymmetric part. In Backus' decomposition three of the harmonic tensors are related to the totally symmetric part, and two are related to the asymmetric part. Is that also the case in Cowin's decomposition? Backus's decomposition is said to be unique, what does this uniqueness mean?

As an assumption in the development of the decomposition of Backus, **E** is first decomposed as a sum of the totally symmetric part and the asymmetric part. Then the decomposition into harmonic tensors is developed. The resulting expression for the harmonic decomposition of **E** presented in (2.23) is arranged as a sum of a totally symmetric part and an asymmetric part. Here H_{ijkl}, H_{ij} and H represent the totally symmetric part, h_{ij} and h represent the asymmetric part. The asymmetric part is thus expressed by means of a second-order and a zeroth-order harmonic tensor.

Is Cowin's decomposition in (2.34) also expressed in two parts as a sum of a totally symmetric part and an asymmetric part with the similar correspondence to $\hat{A}_{ij}, \hat{B}_{ij}, a$, and b as in Backus' expression mentioned above ?

Consider the possible combinations of a 2nd order and a zeroth-order harmonic tensor from Cowin's decomposition, and let us investigate whether the associated contribution to **E** is asymmetric. Let us denote four of the contributions to **E** as follows:

$$\begin{aligned} X^{(1)}_{ijkl} &= a\delta_{ij}\delta_{kl}, & X^{(2)}_{ijkl} &= b[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}], \\ X^{(3)}_{ijkl} &= \delta_{ij}\hat{A}_{kl} + \delta_{kl}\hat{A}_{ij}, & X^{(4)}_{ijkl} &= \delta_{ik}\hat{B}_{jl} + \delta_{jl}\hat{B}_{ik} + \delta_{il}\hat{B}_{jk} + \delta_{jk}\hat{B}_{il}. \end{aligned} \tag{2.37}$$

The following four combinations are the possible contributions to **E** associated with a second-order and a zeroth-order harmonic tensor:

$$X^{(1)}_{ijkl} + X^{(3)}_{ijkl}, \quad X^{(2)}_{ijkl} + X^{(3)}_{ijkl}, \quad X^{(1)}_{ijkl} + X^{(4)}_{ijkl}, \quad X^{(2)}_{ijkl} + X^{(4)}_{ijkl}.$$

For an asymmetric elastic tensor, the following relation is valid:

$$A_{ijkl} + A_{iklj} + A_{iljk} = 0. \tag{2.38}$$

None of the four combinations above, and no other combinations of second- and zeroth-order harmonic tensors from (2.34) will satisfy (2.38). It follows that Cowin's decomposition is not expressed as a sum of a totally symmetric tensor S_{ijkl}, and an asymmetric part A_{ijkl} related to a second-order harmonic tensor and a constant.

Is Cowin's decomposition at all arranged as a totally symmetric part and an asymmetric part? None of the expressions $X^{(1)}_{ijkl}, \ldots$, and no combination of two or more of them are totally symmetric. Suppose that a sum of Z_{ijkl} and one or more of the above-defined expressions are asymmetric. Since the rest cannot be symmetric, $\mathbf{E}$ is not expressed as a sum of a totally symmetric part and an asymmetric part. For example, to show that $X^{(4)}_{ijkl}$ is not totally symmetric, consider

$$X^{(4)}_{ikjl} = \delta_{ij}\hat{B}_{kl} + \delta_{kl}\hat{B}_{ij}, + \delta_{il}\hat{B}_{jk} + \delta_{jk}\hat{B}_{il}.$$

Since $X^{(4)}_{ijkl}$ is different from $X^{(4)}_{ikjl}$, $\mathbf{X}^{(4)}$ is not totally symmetric. None of the expressions $X^{(1)}_{ijkl}, \ldots$ in (2.37), and no combination of two or more of them are asymmetric. Suppose that a sum of Z_{ijkl} and one or more of the above-defined expressions are totally symmetric. Since the rest cannot be asymmetric, $\mathbf{E}$ is not expressed as a sum of a totally symmetric part and an asymmetric part.

Further investigation shows that grouping of terms in (2.34), apart from Z_{ijkl}, makes neither totally symmetric nor asymmetric tensors.

The above discussion shows that Cowin's decomposition is not expressed as a decomposition into totally symmetric and asymmetric tensors, but of course it is possible to do so.

In spite of assuming a different arrangement than Backus in developing the decomposition, Cowin's decomposition can be expressed by means of H_{ij}, H, h_{ij}, and h from Backus' decomposition by means of a linear transformation.

Backus (**1**) has stated that every elastic tensor is expressible in terms of unique harmonic tensors, one of order 4, two of order 2 and two of order 0. But the condition in this decomposition is that the elastic tensor is first decomposed into the totally symmetric part and the asymmetric part. Then the harmonic tensors in (2.27) to (2.31) are unique.

The sum of the contributions associated with the two second-order harmonic tensors in Backus' decomposition is the same as in Cowin's decomposition. The sums of the contributions associated with the two zeroth-order tensors are also the same for the two decompositions. It follows then that the fourth-order tensors in Backus' and Cowin's decompositions must be equal. Thus Cowin could use Backus' explicit expression (2.29) for the fourth-order harmonic tensor.

As an example, the contribution from the two zeroth-order tensors is, according to Cowin's expression in (2.34),

$$e_{ijkl} = \frac{1}{15}(2\mathrm{tr}\,\mathbf{C} - \mathrm{tr}\,\mathbf{V})\delta_{ij}\delta_{kl} + \frac{1}{30}(3\mathrm{tr}\,\mathbf{V} - \mathrm{tr}\,\mathbf{C})[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}]$$

$$= \frac{2}{15}\mathrm{tr}\,\mathbf{C}\,\delta_{ij}\delta_{kl} - \frac{1}{15}\mathrm{tr}\,\mathbf{V}\,\delta_{ij}\delta_{kl} + \frac{1}{10}\mathrm{tr}\,\mathbf{V}\delta_{ik}\delta_{jl} - \frac{1}{30}\mathrm{tr}\,\mathbf{C}\,\delta_{ik}\delta_{jl}$$
$$+\frac{1}{10}\mathrm{tr}\,\mathbf{V}\delta_{il}\delta_{jk} - \frac{1}{30}\mathrm{tr}\,\mathbf{C}\,\delta_{il}\delta_{jk}.$$

Mochizuki **(9)** also presents a decomposition of the elastic tensor into harmonic tensors. In this decomposition the elastic tensor is not decomposed into a totally symmetric tensor and an asymmetric tensor, but by means of two parts where the first part is a fourth-order tensor of 15 independent terms. The second part contains a second-order symmetric tensor and a constant. The fourth-order tensor is not totally symmetric. Each of the two parts is decomposed into harmonic tensors. These harmonic tensors are not expected to be equal to the harmonic tensors in Backus' decomposition.

Mochizuki's decomposition differs also from the decomposition of Backus in another respect. Mochizuki gives the decomposition of the covariant canonical components of the elastic tensor, while Backus uses Cartesian components. See also Phinney and Burridge **(10)** for a discussion of the canonical components.

2.13 Maxwell multipoles

According to Backus, Sylvester's theorem can be expressed as follows. Given any real 3-dimensional homogeneous polynomial of order $q \geq 2$, there exist q real vectors $\mathbf{a}^{(1)}, \ldots, \mathbf{a}^{(q)}$ and a real 3-dimensional homogeneous polynomial of order $q-2$ such that

$$P^{(q)}(r) = (\mathbf{a}^{(1)} \cdot \mathbf{r})(\mathbf{a}^{(2)} \cdot \mathbf{r}) \ldots (\mathbf{a}^{(q)} \cdot \mathbf{r}) + r^2 P^{(q-2)}(r).$$

The vectors $\mathbf{a}^{(1)}, \ldots, \mathbf{a}^{(q)}$ are uniquely determined by $P^{(q)}(r)$ to within multiplication by arbitrary real constants whose product is unity, and $P^{(q-2)}(r)$ is also uniquely determined by $P^{(q)}$. The $(\mathbf{a}^{(1)} \cdot \mathbf{r}), (\mathbf{a}^{(2)} \cdot \mathbf{r}), \ldots$, are scalar products.

Replacing $P^{(q)}(r)$ by any real non-zero homogeneous harmonic polynomial of degree q in three dimensions, we have

$$H^{(q)}(r) = A \prod_{v=0}^{q} (\hat{\mathbf{a}}^{(v)} \cdot \mathbf{r}) + r^2 P^{(q-2)}(r), \qquad (2.39)$$

where $\hat{\mathbf{a}}^{(1)}, \ldots \hat{\mathbf{a}}^{(q)}$ are real unit vectors, and A is a positive constant.

The polynomial $P^{(q-2)}(r)$ and the constant A are uniquely determined by $H^{(q)}(r)$, and the set of directions $(\hat{\mathbf{a}}^{(1)}, \ldots \hat{\mathbf{a}}^{(q)})$ is determined to within an even number of sign changes. That is, we can alter the sign of any two of the unit vectors $\hat{\mathbf{a}}^{(1)}, \ldots$ without altering the product in (2.39). The constant A and the set $(\hat{\mathbf{a}}^{(1)}, \ldots, \hat{\mathbf{a}}^{(q)})$ also uniquely determine $H^{(q)}(r)$ in (2.39).

To each harmonic polynomial corresponds a unique harmonic tensor. Thus, to each harmonic tensor of order q is associated a set of q unit vectors $(\hat{\mathbf{a}}^{(1)}, \ldots \hat{\mathbf{a}}^{(q)})$ and an amplitude A. Equation (2.18) gives the decomposition of a totally symmetric tensor **S**. For the totally symmetric part of an elastic tensor, three sets of unit vectors are associated (to $\mathbf{H}^{(0)}$ corresponds a point). Since the asymmetric part of the elastic tensor can also be expressed by means of totally symmetric tensors, an elastic tensor corresponds to five sets of unit vectors and associated amplitudes.

As an application of the multipoles, let us consider a material with cubic symmetry. Then the geometry of the five sets of unit vectors must be invariant under all rotations that leave the cube invariant. Following the arguments of Backus, no bouquet of two unit vectors can have the symmetry of a cube. If a bouquet of four unit vectors has the symmetries of a cube, the vectors must lie along the principal diagonals of the cube. Thus **E** must have $\mathbf{H}^{(2)} = \mathbf{h}^{(2)} = 0$ for a cubic material. The diagonals in a cube centered in origin, have the directions

$$\mathbf{a}^{(1)} = \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3, \qquad \mathbf{a}^{(2)} = \mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_3,$$

$$\mathbf{a}^{(3)} = \mathbf{e}_1 + \mathbf{e}_2 - \mathbf{e}_3, \qquad \mathbf{a}^{(4)} = \mathbf{e}_1 - \mathbf{e}_2 - \mathbf{e}_3,$$

where $\mathbf{e}_1, \mathbf{e}_2$, and $\mathbf{e}_3$ are unit vectors in x-, y-, and z- direction respectively. From (2.39) we have

$$H^{(4)}(r) = A\prod_{v=0}^{4}(\hat{\mathbf{a}}^{(v)}\cdot\mathbf{r}) + r^2P^{(2)}(r) = A\prod_{v=0}^{4}(\hat{\mathbf{a}}^{(v)}\cdot\mathbf{r}) + r^2\tilde{H}^{(2)}(r) + r^4\tilde{H}^{(0)},$$

since any homogeneous polynomial $P^{(2)}(r)$ can be decomposed by harmonic polynomials. Notice that $\tilde{\mathbf{H}}^{(2)}$ and $\tilde{\mathbf{H}}^{(0)}$ are not the harmonic tensors in the decomposition of **E**.

Substituting for $\mathbf{a}^{(1)}, \mathbf{a}^{(2)}, \mathbf{a}^{(3)}, \mathbf{a}^{(4)}$ and $\mathbf{r} = x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3$ we have

$$\begin{aligned}\mathbf{H}^{(4)}(\mathbf{r}) = \;& A[(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3)\cdot(x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3)] \\ & \times[(\mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_3)\cdot(x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3)] \\ & \times[(\mathbf{e}_1 + \mathbf{e}_2 - \mathbf{e}_3)\cdot(x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3)] \\ & \times[(\mathbf{e}_1 - \mathbf{e}_2 - \mathbf{e}_3)\cdot(x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3)] + r^2\tilde{H}^{(2)}(r) + r^4\tilde{H}^{(0)} \\ = \;& A[x^4 + y^4 + z^4 - 2x^2y^2 - 2x^2z^2 - 2y^2z^2] + r^2\tilde{H}^{(2)}(r) + r^4\tilde{H}^{(0)}\end{aligned}$$

After application of the Laplace operator and (2.15) we have

$$0 = A(4x^2 + 4y^2 + 4z^2) + 14\tilde{H}^{(2)}(r) + 20r^2\tilde{H}^{(0)}$$

or

$$0 = 4r^2A + 14\tilde{H}^{(2)}(r) + 20r^2\tilde{H}^{(0)}. \tag{2.40}$$

Applying the Laplace operator and (2.15) once more gives $0 = A + 5\tilde{H}^{(0)}$ or

$$A = -5\tilde{H}^{(0)}.$$

It follows then that $\tilde{H}^{(2)} = 0$ after substituting for A in (2.40) Let us define $\alpha = 2A/5$ It follows that $\tilde{H}^{(0)} = -A/5 = -\alpha/2$. Then $\mathbf{H}^{(4)}(\mathbf{r})$ becomes

$$\begin{aligned}\mathbf{H}^{(4)}(\mathbf{r}) &= \frac{5\alpha}{2}[x^4 + y^4 + z^4 - 2x^2y^2 - 2x^2z^2 - 2y^2z^2] \\ &\quad -\frac{\alpha}{2}[x^4 + y^4 + z^4 + 2x^2y^2 + 2x^2z^2 + 2y^2z^2] \\ &= 2\alpha[x^4 + y^4 + z^4 - 3x^2y^2 - 3x^2z^2 - 3y^2z^2].\end{aligned}$$

From the polynomial above, we can find the components of the tensor $\mathbf{H}^{(4)}$ from (2.8):

$$H_{1111} = H_{2222} = H_{3333} = \frac{1}{4!}2\alpha(4 \times 3 \times 2) = 2\alpha,$$

$$H_{1122} = H_{1133} = H_{2233} = H_{2323} = H_{1313} = H_{1212} = -\frac{1}{4!}2\alpha(3 \times 2 \times 2) = -\alpha.$$

The rest of the 21 components are equal to zero. Then $\mathbf{H}^{(4)}$ can be displayed as a 6×6 matrix by using the two-index notation:

$$\begin{pmatrix} 2\alpha & -\alpha & -\alpha & 0 & 0 & 0 \\ & 2\alpha & -\alpha & 0 & 0 & 0 \\ & & 2\alpha & 0 & 0 & 0 \\ & & & -\alpha & 0 & 0 \\ & & & & -\alpha & 0 \\ & & & & & -\alpha \end{pmatrix}$$

What remains in the representation of $\mathbf{E}$ is the contribution associated with H and h. Let us denote this contribution by $\mathbf{e}$. Notice that $\mathbf{H}^{(2)} = \mathbf{h}^{(2)} = 0$. From (2.23) we have

$$e_{ijkl} = H[\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] + h[\delta_{ij}\delta_{kl} - \frac{1}{2}\delta_{ik}\delta_{jl} - \frac{1}{2}\delta_{il}\delta_{jk}]$$

which gives

$$\begin{aligned} e_{1111} &= e_{2222} = e_{3333} = 3H, \\ e_{1122} &= e_{1133} = e_{2233} = H + h, \\ e_{2323} &= e_{1313} = e_{1212} = H - \frac{1}{2}h. \end{aligned}$$

The rest of the 21 components of $\mathbf{e}$ are equal to zero. These are also the components for the elastic tensor in the isotropic case since $\mathbf{H}^{(4)} = \mathbf{H}^{(2)} = \mathbf{h}^{(2)} = 0$ in that case.

In the cubic case $\mathbf{E}$ is the sum of $\mathbf{H}^{(4)}$ and $\mathbf{e}$, and can be displayed as

$$\begin{pmatrix} 2\alpha + 3H & -\alpha + H + h & -\alpha + H + h & 0 & 0 & 0 \\ & 2\,\alpha + 3H & -\alpha + H + h & 0 & 0 & 0 \\ & & 2\alpha + 3H & 0 & 0 & 0 \\ & & & -\alpha + H - \frac{h}{2} & 0 & 0 \\ & & & & -\alpha + H - \frac{h}{2} & 0 \\ & & & & & -\alpha + H - \frac{h}{2} \end{pmatrix}$$

or

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ & c_{11} & c_{12} & 0 & 0 & 0 \\ & & c_{11} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{44} & 0 \\ & & & & & c_{44} \end{pmatrix}$$

2.14 Conclusion

Application of Backus' theory to the elasticity tensor is presented. The theory is illustrated by examples, and numerical examples of the harmonic decomposition of the elasticity tensor are given.

Total symmetry is a very important concept in this theory. In a totally symmetric tensor, all tensor components T_{ijkl} with specific indices i, j, k and l are equal regardless the permutation of the indices. In the elastic case it is shown that for the totally symmetric part of a tensor, each component can be expressed by three elastic constants. Backus' definition of totally symmetric tensor satisfies the conditions above.

Cowin **(2)** also defines the totally symmetric part of an elastic tensor. It is shown that this definition does not satisfy the definition given above.

The totally symmetric part of a tensor generate the same homogeneous polynomial as the tensor itself. This is an important fact used in the harmonic decomposition of the elasticity tensor. As an example, the proof is given for a fourth-order tensor. The coefficients in the totally symmetric part of a tensor can be obtained from this homogeneous polynomial. There is a unique totally symmetric tensor generating a given polynomial.

A totally symmetric elastic tensor has 15 independent components instead of 21. The asymmetric part is the difference between the elasticity tensor and the totally symmetric tensor, has six independent components, and elastic symmetry.

When the coordinate system is the symmetry axes, the second-order totally symmetric tensor associated to the asymmetric part of the elasticity tensor is always a diagonal tensor for all symmetry classes apart from monoclinic and triclinic. For the monoclinic case, the 2nd order tensor can be diagonalized by rotating the coordinate system around the symmetry axis. When the elasticity tensor is given by 21 elastic constants, the 2nd order related tensor is not diagonal. By diagonalization of this 2nd order tensor, the elasticity tensor is in a symmetry coordinate system when the eigenvectors are the coordinate axes. The form of the transformed tensor shows which symmetry system we have, and which axes is the symmetry axis. For cubic symmetry, diagonalization do not give the symmetry coordinate system. Maxwell multipoles associated to the fourth order harmonic tensor gives the directions along the diagonals. Then the new coordinate system is known.

A comparison of Backus' decomposition into one fourth-order harmonic tensor, two second-order harmonic tensors and two scalars with Cowin's decomposition is presented. Both decompositions are expressed by means of the dilatational modulus tensor and the Voigt tensor. The two decompositions are different, but unique under quite different conditions. It is also shown that the 4th order harmonic tensors are equal in the two decompositions. Thus Cowin could use Backus' formula for the fourth-order tensor in his theory. Cowin does not have a general expression for the fourth-order tensor, but Backus' explicit expression can be used in Cowin's decomposition.

Acknowledgements

This work was done at the University of Utrecht, Department of Exploration Geophysics. I wish to thank Professor K. Helbig for advice and discussions. I would also like to thank one of the referees, Professor Stephen Cowin, for fruitful discussions about parts of the manuscript.

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Chapter 3

Decomposition of the anisotropic elastic tensor in base tensors

Abstract

The elastic tensor generally has 21 nonvanishing stiffnesses. In this article a decomposition of the elastic tensors into 21 orthonormal base tensors in a 21-dimensional vector space is presented. The elements in the vector space are tensors and the base tensors are derived from harmonic tensors (see Backus, 1970). Each elastic tensor can be expressed as a unique linear combination of the 21 base tensors.

In this vector space a metric is defined. By means of the metric, deviation from spesific symmetry classes is defined. For the different symmetry classes, monoclinic, orthorhombic etc., the decomposition of the elastic tensor into the 21 base tensors is presented. The decomposition generally depends on the coordinate system to which the elastic tensor is referred.

3.1 Introduction

In an arbitrary coordinate system, all elastic tensors except isotropic have 21 nonvanishing stiffnesses. If the medium has some kind of symmetry higher than triclinic, the problem of establishing the symmetry can be treated by means of harmonic decomposition of the elastic tensor. Several publications (Backus, 1970; Mochizuki, 1988;

This chapter has been published as:
R. Baerheim and K. Helbig, *Decomposition of the anisotropic elastic tensor in base tensors*, Canadian Journal of Exploration Geophysics, Vol. 29. No. 1, p. 41-50, 1993

Cowin, 1989) present decomposition of the elastic tensor into harmonic tensors. The harmonic tensors are of rank four, two and zero. By means of this decomposition, the symmetry class and the symmetry coordinate system can be determined. A harmonic tensor is totally symmetric, and traceless with respect to all pairs of indices. In a totally symmetric tensor, all tensor components T_{ijkl} with specific indices i, j, k and l are equal for all permutations of the indices.

An orthonormal basis in the 21-dimensional vector space of elastic tensors is given. The orthonormal base tensors are created from harmonic tensors of rank four, two and zero.

A tensor is a physical entity. However, in the literature, tensor $\mathbf{T}$ is normally used to denote the representation relative a coordinate system, the components of which must transform from one coordinate system to another by the rule: $T'_{i_1 i_2 \ldots} = \alpha_{i_1 k_1} \alpha_{i_2 k_2} \ldots T_{k_1 k_2 \ldots}$, where $\alpha_{i_v k_v}$ is the cosine between the new i_v -axis and the old k_v -axis.

In this article, a tensor denotes the representation mentioned above, i.e., its array of components in a given coordinate system. The inner product is a scalar and has a physical meaning. It is invariant against coordinate transformation.

The definition of a metric increases the possibilities of performing numerical calculations. One example where the notion of inner product is useful is for the quantification of deviation from symmetry class. This is also treated in this article.

3.2 Introducing base tensors and metric in the vector space of elastic tensors

Let us start by defining a hierarchically symmetric tensor $\mathbf{E}$ as a tensor of rank four and dimension 3, which satisfies

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}. \tag{3.1}$$

The tensor is elastic if the hierarchically symmetric tensor is positive definite, i.e., $\epsilon_{ij}\,\epsilon_{kl}\,E_{ijkl} > 0$ for all ϵ_{ij}. The hierarchically symmetric tensor can be decomposed into harmonic tensors of rank four, two and zero (see Backus, 1970). The dimension of the vector space consisting of harmonic tensors of rank q is $2q + 1$.

In the following, a set of base tensors is created by means of harmonic tensors of rank four, two and zero. Harmonic tensors are uniquely related to spherical harmonic polynomials via the formula:

$$H_{i_1,\ldots,i_q} = \frac{1}{q!} \partial_{i_1 \ldots i_q} H(r), \tag{3.2}$$

where $\partial_{i_1 \ldots i_q}$ denotes the qth-order partial derivative with respect to $r_{i_1}, \ldots, r_{i_q}$. Equation (3.2) is a general formula which relates homogeneos polynomials to unique totally symmetric tensors (see Ch. 2 where the formula is employed for $q = 4$). Harmonic tensors of rank two and zero are related to a totally symmetric fourth rank tensor S_{ijkl} and a hierarchically symmetric tensor A_{ijkl} where the totally symmetric part is subtracted. Let the symbol A_{ijkl} stand for a hierarchically symmetric tensor with vanishing totally symmetric part, related to a specific general hierarchically symmetric tensor by $E_{ijkl} = S_{ijkl} + A_{ijkl}$.

The relation between a harmonic tensor of rank zero, i.e., a scalar, and the two created tensors S_{ijkl} and A_{ijkl} is given by (see Backus, 1970):

$$S_{ijkl} = H(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{3.3}$$

and

$$A_{ijkl} = H(\delta_{ij}\delta_{kl} - \frac{1}{2}\delta_{ik}\delta_{jl} - \frac{1}{2}\delta_{il}\delta_{jk}). \tag{3.4}$$

An alternative, and perhaps more instructive, way to obtain equations (3.3) and (3.4) is the following: if H is given, define a hierarchically symmetric tensor $E_{ijkl} = 3H\delta_{ij}\delta_{kl}$. The totally symmetric part is:

$$\frac{1}{3}(E_{ijkl} + E_{ikjl} + E_{iljk}) = H(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),$$

which is the same as the expression in (3.3). The non-totally symmetric part of E_{ijkl} is:

$$\begin{aligned} A_{ijkl} = E_{ijkl} - S_{ijkl} &= 3H\delta_{ij}\delta_{kl} - H(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ &= H(2\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}), \end{aligned}$$

which, except for a factor 2, is equal to equation (3.4).

Harmonic tensors of rank 2 are related to hierarchically symmetric tensors by

$$S_{ijkl} = \delta_{ij}H_{kl} + \delta_{kl}H_{ij} + \delta_{ik}H_{jl} + \delta_{jl}H_{ik} + \delta_{il}H_{jk} + \delta_{jk}H_{il}, \tag{3.5}$$

which is totally symmetric, and

$$A_{ijkl} = \delta_{ij}H_{kl} + \delta_{kl}H_{ij} - \frac{1}{2}\delta_{ik}H_{jl} - \frac{1}{2}\delta_{jl}H_{ik} - \frac{1}{2}\delta_{il}H_{jk} - \frac{1}{2}\delta_{jk}H_{il} \tag{3.6}$$

which is non-totally symmetric.

It is shown later that all the hierarchically symmetric tensors in equations (3.3), (3.4), (3.5) and (3.6) are orthogonal.

An alternative way of obtaining equations (3.5) and (3.6) is: given a harmonic tensor H_{ij} of rank 2, define the following hierarchically symmetric tensor:

$$E_{ijkl} = \frac{1}{2}(\delta_{ij}H_{kl} + \delta_{kl}H_{ij}).$$

The totally symmetric part is:

$$E_{ijkl} = \frac{1}{3}(E_{ijkl} + E_{ikjl} + E_{iljk})$$

$$= \frac{1}{6}(\delta_{ij}H_{kl} + \delta_{kl}H_{ij} + \delta_{ik}H_{jl} + \delta_{jl}H_{ik} + \delta_{il}H_{jk} + \delta_{jk}H_{il}),$$

which is the same as equation (3.5) except for the factor $\frac{1}{6}$. We could also arrive at this expression by calculating the totally symmetric part of the product between Kronecker delta and a harmonic tensor of rank two. This is equal to the totally symmetric part $\frac{1}{3}(E_{ijkl} + E_{ikjl} + E_{iljk})$ of a hierarchically symmetric tensor E_{ijkl} if $E_{ijkl} = \frac{1}{2}(\delta_{ij}H_{kl} + \delta_{kl}H_{ij})$. The non totally symmetric part of E_{ijkl} is:

$$A_{ijkl} = E_{ijkl} - S_{ijkl}$$

$$= \frac{1}{3}(\delta_{ij}H_{kl} + \delta_{kl}H_{ij} - \frac{1}{2}\delta_{ik}H_{jl} - \frac{1}{2}\delta_{jl}H_{ik} - \frac{1}{2}\delta_{il}H_{jk} - \frac{1}{2}\delta_{jk}H_{il}),$$

which is the same as equation (3.6) except for the factor $\frac{1}{3}$.

The totally symmetric tensors and non-totally symmetric tensors defined above are used to define a basis in the vector space of hierarchically symmetric tensors.

The vector space of harmonic tensors of rank zero has dimension one, so there is one independent base tensor. To this vector space two hierarchically symmetric tensors, one totally symmetric and one non-totally symmetric, are related via equations (3.3) and (3.4).

The five base harmonic tensors of rank two are related to five totally symmetric and five non-totally symmetric fourth rank tensors.

The nine base harmonic tensors of rank four are totally symmetric and, therefore, also hierarchically symmetric. The 21 elastic tensors created in this way will be shown to form an orthogonal set of tensors in the 21-dimensional vector space of hierarchically symmetric tensors. They are therefore linear independent and, if normalized, form a set of base vectors in the 21-dimensional vector space (see Halmos, 1958). Each hierarchically symmetric tensor can thus be expressed in only one way as a linear combination of the 21 base tensors.

The inner product of two tensors $\mathbf{T}$ and $\mathbf{U}$ in the vectorspace is defined as $(\mathbf{T},\mathbf{U}) = T_{ijkl}U_{ijkl}$, and the norm of a tensor $\mathbf{T}$ is $\sqrt{(\mathbf{T},\mathbf{T})} = \sqrt{T_{ijkl}T_{ijkl}}$. In the following, the 21 base tensors are presented.

Rank 0:

Harmonic polynomial: $H(r)^{(0,0,C)}$ = solid spherical harmonic of degree zero = 1.
Related harmonic tensor: $H^{(0,0,C)} = 1$ (see (A-27)).
The derived totally symmetric fourth-rank tensor from equation (3.3) is:

$$S_{ijkl} = (\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \quad (3.7)$$

With indices of the hierarchically symmetric tensor organized according to the following scheme

$$
\begin{array}{ccc|ccc|ccc}
1111 & 1112 & 1113 & 1211 & 1212 & 1213 & 1311 & 1312 & 1313 \\
1121 & 1122 & 1123 & 1221 & 1222 & 1223 & 1321 & 1322 & 1323 \\
1131 & 1132 & 1133 & 1231 & 1232 & 1233 & 1331 & 1332 & 1333 \\
\hline
2111 & 2112 & 2113 & 2211 & 2212 & 2213 & 2311 & 2312 & 2313 \\
2121 & 2122 & 2123 & 2221 & 2222 & 2223 & 2321 & 2322 & 2323 \\
2131 & 2132 & 2133 & 2231 & 2232 & 2233 & 2331 & 2332 & 2333 \\
\hline
3111 & 3112 & 3113 & 3211 & 3212 & 3213 & 3311 & 3312 & 3313 \\
3121 & 3122 & 3123 & 3221 & 3222 & 3223 & 3321 & 3322 & 3323 \\
3131 & 3132 & 3133 & 3231 & 3232 & 3233 & 3331 & 3332 & 3333
\end{array},
$$

the totally symmetric tensor (3.7) has the components:

$$
\begin{array}{ccc|ccc|ccc}
3 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
\hline
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\
\hline
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 3
\end{array}.
$$

In matrix form, the normalised base tensor is given as:

$$
\mathbf{e}^{(1)} = \frac{1}{3\sqrt{5}} \begin{pmatrix} 3 & 1 & 1 & 0 & 0 & 0 \\ & 3 & 1 & 0 & 0 & 0 \\ & & 3 & 0 & 0 & 0 \\ & & & 1 & 0 & 0 \\ & & & & 1 & 0 \\ & & & & & 1 \end{pmatrix} \tag{3.8}
$$

From equation (3.4) the derived non-totally symmetric tensor is given by

$$
A_{ijkl} = (\delta_{ij}\delta_{kl} - \frac{1}{2}\delta_{ik}\delta_{jl} - \frac{1}{2}\delta_{il}\delta_{jk}). \tag{3.9}
$$

and has the components

$$
\begin{array}{ccc|ccc|ccc}
0 & 0 & 0 & 0 & -0.5 & 0 & 0 & 0 & -0.5 \\
0 & 1 & 0 & -0.5 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & -0.5 & 0 & 0 \\
\hline
0 & -0.5 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
-0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.5 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & -0.5 & 0 \\
\hline
0 & 0 & 0.5 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -0.5 & 0 & 1 & 0 \\
-0.5 & 0 & 0 & 0 & -0.5 & 0 & 0 & 0 & 0
\end{array},
$$

and in matrix form the normalised base tensor $\mathbf{e}^{(2)}$ is given as:

$$
\mathbf{e}^{(2)} = \frac{1}{3}\begin{pmatrix}
0 & 1 & 1 & 0 & 0 & 0 \\
 & 0 & 1 & 0 & 0 & 0 \\
 & & 0 & 0 & 0 & 0 \\
 & & & -0.5 & 0 & 0 \\
 & & & & -0.5 & 0 \\
 & & & & & -0.5
\end{pmatrix} \tag{3.10}
$$

The normalising factors are explained in more detail in the next section.

Rank 2:

From equation (3.5) the totally symmetric fourth-rank tensor related to a second-rank harmonic tensor H_{ij} is given by:

$$
S_{ijkl} = \delta_{ij}H_{kl} + \delta_{kl}H_{ij} + \delta_{ik}H_{jl} + \delta_{jl}H_{ik} + \delta_{il}H_{jk} + \delta_{jk}H_{il}. \tag{3.11}
$$

From equation (3.6) the non-totally symmetric tensor is given by

$$
A_{ijkl} = \delta_{ij}H_{kl} + \delta_{kl}H_{ij} - \frac{1}{2}\delta_{ik}H_{jl} - \frac{1}{2}\delta_{jl}H_{ik} - \frac{1}{2}\delta_{il}H_{jk} - \frac{1}{2}\delta_{jk}H_{il}. \tag{3.12}
$$

The harmonic polynomial $H(r)^{(2,0)}$ and related tensor is given respectively by:

$$
H(r)^{(2,0)} = x^2 + y^2 - 2z^2 \tag{3.13}
$$

and

$$
H^{(2,0)} = \begin{pmatrix}
1 & 0 & 0 \\
 & 1 & 0 \\
 & & -2
\end{pmatrix} \tag{3.14}
$$

where (3.13) corresponds to (A-31). The two base tensors $\mathbf{e}^{(3)}$ and $\mathbf{e}^{(4)}$ generated by the above harmonic tensor by applying equations (3.11) and (3.12) together with normalizing factors are given in the appendix of this chapter.

The next four harmonic polynomials and related tensors are as follows:

$$H(r)^{(2,1,C)} = 2xz, \qquad H^{(2,1,C)} = \begin{pmatrix} 0 & 0 & 1 \\ & 0 & 0 \\ & & 0 \end{pmatrix} \tag{3.15}$$

$$H(r)^{(2,1,S)} = 2yz, \qquad H^{(2,1,S)} = \begin{pmatrix} 0 & 0 & 0 \\ & 0 & 1 \\ & & 0 \end{pmatrix} \tag{3.16}$$

$$H(r)^{(2,2,C)} = x^2 - y^2, \qquad H^{(2,2,C)} = \begin{pmatrix} 1 & 0 & 0 \\ & -1 & 0 \\ & & 0 \end{pmatrix} \tag{3.17}$$

$$H(r)^{(2,2,S)} = 2xy, \qquad H^{(2,2,S)} = \begin{pmatrix} 0 & 1 & 0 \\ & 0 & 0 \\ & & 0 \end{pmatrix}. \tag{3.18}$$

where the polynomials in (3.15) - (3.18) correspond to (A-32) - (A-35). The four totally symmetric and four non-totally symmetric tensors generated from (3.11) and (3.12), together with normalizing factors, are denoted $\mathbf{e}^{(5)} \ldots \mathbf{e}^{(12)}$ and are given in the appendix of this chapter.

Rank 4:

The nine different harmonic polynomials of rank four are given below (see Appendix). The related tensors calculated from equation (3.2) are totally symmetric fourth rank tensors. They are denoted $\mathbf{e}^{(13)} \ldots \mathbf{e}^{(21)}$ and are given in the appendix of this chapter.

$$H(r)^{(4,0)} = 3x^4 + 3y^4 + 8z^4 - 24x^2z^2 - 24y^2z^2 + 6x^2y^2, \tag{3.19}$$

$$H(r)^{(4,1,C)} = -16xz^3 + 12x^3z + 12xy^2z, \tag{3.20}$$

$$H(r)^{(4,1,S)} = -16yz^3 + 12y^3z + 12x^2yz, \tag{3.21}$$

$$H(r)^{(4,2,C)} = x^4 - y^4 - 6x^2z^2 + 6y^2z^2, \tag{3.22}$$

$$H(r)^{(4,2,S)} = 4x^3y + 4xy^3 - 24xyz^2, \tag{3.23}$$

$$H(r)^{(4,3,C)} = 4x^3z - 12xy^2z, \tag{3.24}$$

$$H(r)^{(4,3,S)} = 4y^3z - 12x^2yz, \tag{3.25}$$

$$H(r)^{(4,4,C)} = x^4 + y^4 - 6x^2y^2, \tag{3.26}$$

$$H(r)^{(4,4,S)} = 4x^3y - 4xy^3, \tag{3.27}$$

3.3 Orthonormality of base tensors

The definition of the 21 base tensors is based on Backus' decomposition of the vector space of fourth-rank tensors in three dimensions. The subspace of hierarchically symmetric tensors is decomposed into subspaces of different symmetries. It is argued that the subspaces are orthogonal, but it is not proved. Between each of those subspaces and subspaces of harmonic tensors, homomorphisms are defined. It is stated that the homomorphisms are isomorphisms, but the proof is omitted. An isomorhpism is a one to one mapping from one space onto another space. The existence of an isomorphism between two vector spaces implies the same dimension of the vector spaces. Since the subspaces of hierarchically symmetric spaces are orthogonal, the harmonic representations of hierarchically symmetric tensors for each of the subspaces are orthogonal.

We will now show that the base tensors $e^{(i)}$ form an orthonormal set of tensors. The norm of the tensors will also be given.

Let us start with the two base tensors related to the harmonic tensor of rank zero. Equations (3.7) and (3.9) give the expression for the totally symmetric and the non-totally symmetric tensor. If two tensors are orthogonal, their inner product must vanish. The inner product of the two hierarchcally symmetric tensors related to the harmonic tensor of rank 0 is:

$$S_{ijkl}A_{ijkl} = H^2(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})(\delta_{ij}\delta_{kl} - \frac{1}{2}\delta_{ik}\delta_{jl} - \frac{1}{2}\delta_{il}\delta_{jk}) = 0,$$

where $\delta_{ii} = 3$ is used. This shows that S_{ijkl} and A_{ijkl} are orthogonal according to definition.

Now the norm of the two tensors S_{ijkl} and A_{ijkl} will be calculated. The inner product $S_{ijkl}S_{ijkl}$ is given by (noting that $H = 1$ in (3.7) and (3.9)):

$$S_{ijkl}S_{ijkl} = (\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) = 45.$$

The norm of **S** is then

$$\sqrt{S_{ijkl}S_{ijkl}} = \sqrt{45} = 3\sqrt{5}.$$

Similarly, the norm of A_{ijkl} is given by the following inner-product

$$A_{ijkl}A_{ijkl} = (\delta_{ij}\delta_{kl} - \frac{1}{2}\delta_{ik}\delta_{jl} - \frac{1}{2}\delta_{il}\delta_{jk})(\delta_{ij}\delta_{kl} - \frac{1}{2}\delta_{ik}\delta_{jl} - \frac{1}{2}\delta_{il}\delta_{jk}) = 9.$$

Thus, the norm of **A** is

$$\sqrt{A_{ijkl}A_{ijkl}} = 3.$$

For the norm of the base tensors to be one, the factors $1/(3\sqrt{5})$ and $1/3$ occur in equations (3.8) and (3.10).

For rank 2, the totally symmetric tensor and the non-totally symmetric tensor is given by equations (3.11) and (3.12). To show that two different totally symmetric tensors S^a_{ijkl} and S^b_{ijkl} are orthogonal, the inner product $S^a_{ijkl}S^b_{ijkl}$ is calculated:

$$\begin{aligned} S^a_{ijkl}S^b_{ijkl} &= (\delta_{ij}H^a_{kl} + \delta_{kl}H^a_{ij} + \delta_{ik}H^a_{jl} + \delta_{jl}H^a_{ik} + \delta_{il}H^a_{jk} + \delta_{jk}H^a_{il}) \\ &\quad \cdot(\delta_{ij}H^b_{kl} + \delta_{kl}H^b_{ij} + \delta_{ik}H^b_{jl} + \delta_{jl}H^b_{ik} + \delta_{il}H^b_{jk} + \delta_{jk}H^b_{il}) \\ &= 3H^a_{kl}H^b_{kl} + H^a_{ii}H^b_{kk} + 4H^a_{ij}H^b_{ij} + H^a_{kk}H^b_{ii} + \cdots + 3H^a_{il}H^b_{il}. \end{aligned}$$

Since H_{ij} is traceless, and H^a_{ij} and H^b_{ij} are orthogonal symmetric tensors, we have

$$6(3H^a_{kl}H^b_{kl} + 4H^a_{ij}H^b_{ij}) = 42H^a_{ij}H^b_{ij} = 0$$

when $a \neq b$. It is then shown that totally symmetric fourth-rank tensors related to different second-rank harmonic tensors are orthogonal.

When $a = b$,

$$S_{ijkl}S_{ijkl} = 42H_{ij}H_{ij},$$

and the norm of S_{ijkl} is

$$\sqrt{S_{ijkl}\,S_{ijkl}} = \sqrt{42H_{ij}H_{ij}}. \tag{3.28}$$

The inner product of two different non-totally symmetric tensors generated by second-rank harmonic tensors is:

$$\begin{aligned} A^a_{ijkl}A^b_{ijkl} &= (\delta_{ij}H^a_{kl} + \delta_{kl}H^a_{ij} - \frac{1}{2}\delta_{ik}H^a_{jl} - \frac{1}{2}\delta_{jl}H^a_{ik} - \frac{1}{2}\delta_{il}H^a_{jk} - \frac{1}{2}\delta_{jk}H^a_{il}) \\ &\quad \cdot(\delta_{ij}H^b_{kl} + \delta_{kl}H^b_{ij} - \frac{1}{2}\delta_{ik}H^b_{jl} - \frac{1}{2}\delta_{jl}H^b_{ik} - \frac{1}{2}\delta_{il}H^b_{jk} - \frac{1}{2}\delta_{jk}H^b_{il}) \end{aligned}$$

Calculations similar to the calculations performed for the totally symmetric tensor above gives

$$A^a_{ijkl}A^b_{ijkl} = 3H^a_{ij}H^b_{ij}.$$

This is equal to zero when $a \neq b$. Thus the orthogonality is proved. The norm of A_{ijkl} is then given by

$$\sqrt{A_{ijkl}\,A_{ijkl}} = \sqrt{3H_{ij}H_{ij}}. \tag{3.29}$$

The base tensors $\mathbf{e}^{(3)} \ldots \mathbf{e}^{(12)}$ are equal to the tensors generated by equations (3.11) and (3.12) divided by the norm given by (3.28) or (3.29).

To show that a totally symmetric fourth-rank tensor and a non-totally symmetric fourth-rank tensor generated by second-rank harmonic tensors are orthogonal, the inner product of S_{ijkl} and A_{ijkl} will be calculated:

$$S_{ijkl}A_{ijkl} = (\delta_{ij}H^a_{kl} + \delta_{kl}H^a_{ij} + \delta_{ik}H^a_{jl} + \delta_{jl}H^a_{ik} + \delta_{il}H^a_{jk} + \delta_{jk}H^a_{il})$$

$$\cdot(\delta_{ij}H^a_{kl} + \delta_{kl}H^a_{ij} - \frac{1}{2}\delta_{ik}H^a_{jl} - \frac{1}{2}\delta_{jl}H^a_{ik} - \frac{1}{2}\delta_{il}H^a_{jk} - \frac{1}{2}\delta_{jk}H^a_{il})$$

After performing the multiplications and using the properties of the Kronecker delta, we get zero.

For the fourth rank harmonic tensors, we have to evaluate all inner products that can be formed with the nine harmonic tensors. Also the norm of each of the nine harmonic tensors is easily found by calculating the expression $\sqrt{H_{ijkl}H_{ijkl}}$.

To calculate the inner product of two hierarchically symmetric tensors T_{ijkl} and U_{ijkl} by using the matrix representation, the following formula gives the correct value:

$$\begin{aligned} &T_{11}U_{11} + T_{22}U_{22} + T_{33}U_{33} + 2(T_{23}U_{23} + T_{13}U_{13} + T_{12}U_{12}) \\ &+4(T_{44}U_{44} + T_{55}U_{55} + T_{66}U_{66} + T_{14}U_{14} + T_{25}U_{25} + T_{36}U_{36}) \\ &+4(T_{34}U_{34} + T_{15}U_{15} + T_{26}U_{26} + T_{24}U_{24} + T_{35}U_{35} + T_{16}U_{16}) \\ &\qquad\qquad +8(T_{56}U_{56} + T_{46}U_{46} + T_{45}U_{45}). \end{aligned} \tag{3.30}$$

See also Helbig(1993) for norm preserving mapping from hierarchically symmetric tensors to matrix representation. It can be shown that orthogonality is satisfied.

3.4 Symmetry classes

In the following, the stiffness tensor for the different symmetry classes is given in matrix form. In traditional presentation of trigonal and tetragonal symmetry, (see for instance Musgrave, 1970), the number of independent stiffnesses is 7. By proper rotation about the symmetry axis, the number of independent stiffnesses can be reduced from 7 to 6. For monoclinic symmetry, the number of independent stiffnesses can be reduced from 13 to 12 (see Helbig, 1994). Let us start by presenting the different symmetry classes organized in groups according to the scheme in Fig.3.1. In each group the symmetry classes belong to the same subsystem with respect to symmetry. Ranged in order of higher symmetry, let monoclinic, orthorhombic, tetragonal, cubic and isotropic belong to group 1, and monoclinic, trigonal, hexagonal and isotropic symmetry belong to group 2. For group 1, let the 1,2- plane be the symmetry plane for monoclinic and tetragonal system. For group 2, let the 2,3- plane be the symmetry plane for monoclinic and trigonal symmetry. Then the hexagonal symmetry is seen to be a subsystem of tetragonal as well as of trigonal symmetry when represented with 3-axis as symmetry axis.

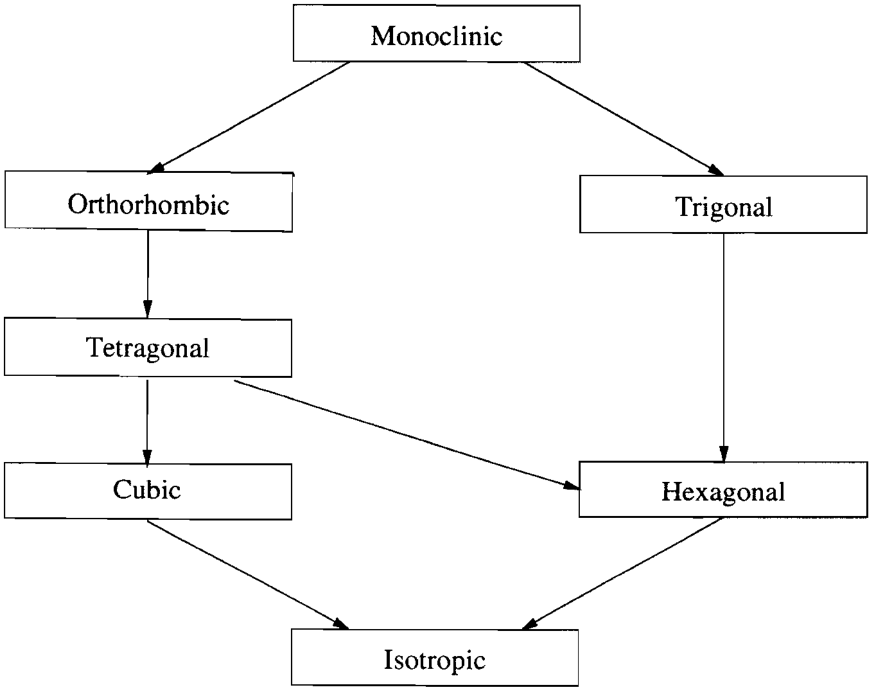

Figure 3.1: The symmetry classes of elastic tensors organized in subsystems of symmetry

Elastic tensors in matrix form for symmetry group 1: the 1,2-plane is the symmetry plane for monoclinic and tetragonal symmetry. For hexagonal symmetry, the 3-axis is the symmetry axis.

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ & c_{22} & c_{23} & 0 & 0 & c_{26} \\ & & c_{33} & 0 & 0 & c_{36} \\ & & & c_{44} & c_{45} & 0 \\ & & & & c_{55} & 0 \\ & & & & & c_{66} \end{pmatrix} \quad \text{Monoclinic}$$

c_{36} or c_{45} can be removed by a rotation about the 3-axis.

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{22} & c_{23} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{55} & 0 \\ & & & & & c_{66} \end{pmatrix} \quad \text{Orthorhombic}$$

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{11} & c_{13} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{44} & 0 \\ & & & & & c_{66} \end{pmatrix} \quad \text{Tetragonal}$$

where $c_{16} = c_{26} = 0$ by rotation about the 3-axis.

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ & c_{11} & c_{12} & 0 & 0 & 0 \\ & & c_{11} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{44} & 0 \\ & & & & & c_{44} \end{pmatrix} \quad \text{Cubic}$$

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ & c_{11} & c_{12} & 0 & 0 & 0 \\ & & c_{11} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{44} & 0 \\ & & & & & c_{44} \end{pmatrix} \quad \text{Isotropic}$$

$$c_{44} = \frac{c_{11} - c_{12}}{2}$$

For group 2, let the 2,3-plane be the symmetry plane for monoclinic and trigonal symmetry. With the 3-axis the symmetry axis for hexagonal symmetry, we get the following matrix representation for group 2:

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ & c_{22} & c_{23} & c_{24} & 0 & 0 \\ & & c_{33} & c_{34} & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{55} & c_{56} \\ & & & & & c_{66} \end{pmatrix} \quad \text{Monoclinic}$$

c_{14} or c_{56} can be removed by a rotation about the 1-axis.

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{44} & c_{14} \\ & & & & & c_{66} \end{pmatrix} \quad \text{Trigonal}$$

$$c_{66} = \frac{c_{11} - c_{12}}{2}$$

where $c_{15} = c_{25} = c_{46} = 0$ by rotation about the 3-axis.

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{11} & c_{13} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{44} & 0 \\ & & & & & c_{66} \end{pmatrix} \quad \text{Hexagonal}$$

$$c_{66} = \frac{c_{11} - c_{12}}{2}$$

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ & c_{11} & c_{12} & 0 & 0 & 0 \\ & & c_{11} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & & & & c_{44} & 0 \\ & & & & & c_{44} \end{pmatrix} \quad \text{Isotropic}$$

$$c_{44} = \frac{c_{11} - c_{12}}{2}$$

3.5 Decomposition of symmetric elastic tensor into base tensors

In the following, a decomposition of the hierarchically symmetric tensor into base tensors is presented. The tensor is represented as a linear combination of the 21 base tensors.

Generally, the hierarchically symmetric tensor $\mathbf{E}$ is expressed by

$$\mathbf{E} = \sum_{i=1}^{21} a_i \mathbf{e}^{(i)}, \tag{3.31}$$

where a_i and $\mathbf{e}^{(i)}$ are the coefficients and base tensors, respectively. To find the coefficient a_j, multiply equation (3.31) by $\mathbf{e}^{(j)}$ (calculate the innerproduct):

$$\mathbf{E}\mathbf{e}^{(j)} = \sum_{i=1}^{21} a_i \mathbf{e}^{(i)} \mathbf{e}^{(j)}.$$

Since $\mathbf{e}^{(i)}$ form an orthonormal set, we get

$$a_j = \mathbf{E}\mathbf{e}^{(j)}. \tag{3.32}$$

Tables 3.1 and 3.2 give the decomposition into base tensors for different symmetry classes when the elastic constants are referred to a symmetry coordinate system (see previous section). Generally, the decomposition depends on the orientation of the coordinate system; see, for instance, the decomposition of monoclinic symmetry and the discussion of Table 3.3.

Symmetry class	$e^{(1)}$	$e^{(2)}$	$e^{(3)}$	$e^{(4)}$	$e^{(5)}$	$e^{(6)}$	$e^{(7)}$	$e^{(8)}$	$e^{(9)}$	$e^{(10)}$	$e^{(11)}$	$e^{(12)}$	$e^{(13)}$	$e^{(14)}$	$e^{(15)}$	$e^{(16)}$	$e^{(17)}$	$e^{(18)}$	$e^{(19)}$	$e^{(20)}$	$e^{(21)}$
									Basis Tensors												
Monoclinic	*	*	*	*					*	*	*	*	*			*	*			*	*
Orthorhombic	*	*	*	*					*	*			*			*				*	
Tetrag. (6 const.) ($C_{16} = C_{26} = 0$)	*	*	*	*									*							*	
Cubic	*	*											*							*	
Isotropic	*	*																			

Table 3.1: Decomposition into base tensors for symmetry classes in group 1. The elastic tensors are referred to a coordinate system where the 1,2 -plane is the symmetry plane for monoclinic and tetragonal symmetry. Base tensors $e^{(1)}$ and $e^{(2)}$ are created from solid spherical harmonics of rank zero. The ten tensors $e^{(3)}$ to $e^{(12)}$ and the nine tensors $e^{(13)}$ to $e^{(21)}$ are created from solid spherical harmonics of rank two and four, respectively.

Symmetry class	$e^{(1)}$	$e^{(2)}$	$e^{(3)}$	$e^{(4)}$	$e^{(5)}$	$e^{(6)}$	$e^{(7)}$	$e^{(8)}$	$e^{(9)}$	$e^{(10)}$	$e^{(11)}$	$e^{(12)}$	$e^{(13)}$	$e^{(14)}$	$e^{(15)}$	$e^{(16)}$	$e^{(17)}$	$e^{(18)}$	$e^{(19)}$	$e^{(20)}$	$e^{(21)}$
	Basis Tensors																				
Monoclinic	*	*	*	*			*	*	*	*			*		*	*			*	*	
Trig. (6 const.) ($C_{15} = C_{25} = C_{46} = 0$)	*	*	*	*									*			*			*		
Hexagonal	*	*	*	*									*								
Isotropic	*	*																			

Table 3.2: Decomposition into base tensors for symmetry classes in group 2. The elastic tensors are referred to a coordinate system where the 2,3 -plane is the symmetry plane for monoclinic and trigonal symmetry. For hexagonal symmetry, the 3 -axis is the symmetry axis. Base tensors $e^{(1)}$ and $e^{(2)}$ are created fron solid spherical harmonics of rank zero. The ten tensors $e^{(3)}$ to $e^{(12)}$ and the nine tensors $e^{(13)}$ to $e^{(21)}$ are created from solid spherical harmonics of rank two and four, respectively.

	Basis Tensors																				
Symmetry class	$e^{(1)}$	$e^{(2)}$	$e^{(3)}$	$e^{(4)}$	$e^{(5)}$	$e^{(6)}$	$e^{(7)}$	$e^{(8)}$	$e^{(9)}$	$e^{(10)}$	$e^{(11)}$	$e^{(12)}$	$e^{(13)}$	$e^{(14)}$	$e^{(15)}$	$e^{(16)}$	$e^{(17)}$	$e^{(18)}$	$e^{(19)}$	$e^{(20)}$	$e^{(21)}$
(2,3) Monoclinic	*	*	*	*			*	*	*	*			*		*	*			*	*	
(1,3) Monoclinic	*	*	*	*	*	*			*	*			*	*		*		*		*	
(1,2) Monoclinic	*	*	*	*					*	*	*	*	*			*	*			*	*
Orthorhombic	*	*	*	*					*	*			*			*				*	
(2,3) Tetragonal	*	*	*	*					*	*			*		*	*			*	*	
(1,3) Tetragonal	*	*	*	*					*	*			*			*				*	
(1,2) Tetragonal	*	*	*	*									*							*	
(2,3) Trigonal	*	*	*	*									*			*			*		
(1,3) Trigonal	*	*	*	*					*	*			*	*		*		*		*	
(1,2) Trigonal	*	*	*	*					*	*			*			*	*			*	*
(I) Hexagonal	*	*	*	*					*	*			*			*				*	
(II) Hexagonal	*	*	*	*					*	*			*			*				*	
(III) Hexagonal	*	*	*	*									*								

Table 3.3: Decomposition into base tensors for symmetry classes referring to three different symmetry coordinate systems. (2,3), (1,3) and (1,2) stand for symmetry plane in coordinate planes (2,3), (1,3) and (1,2), respectively. (I), (II) and (III) stand for symmetry axis parallel to 1-, 2 and 3- coordinate axis, respectively. The decomposition for orthorhombic as well as for cubic is independent of the symmetry coordinate system.

For isotropic symmetry, only a_1 and a_2 are different from zero. We also notice that $\mathbf{e}^{(1)}$ and $\mathbf{e}^{(2)}$ are the only base tensors with isotropic symmetry.

For cubic symmetry a_1, a_2, a_{13} and a_{20} are different from zero. The coefficients are given as:

$$a_1 = (3c_{11} + 2c_{12} + 4c_{44})\frac{\sqrt{5}}{5}, \qquad a_2 = 2(c_{12} - c_{44})$$

and

$$a_{13} = \frac{\sqrt{7}}{5}a_{20} = \frac{1}{\sqrt{2}}(c_{11} - c_{12} - 2c_{44}).$$

This means that the hierarchically symmetric tensor for cubic symmetry can be decomposed by means of $\mathbf{e}^{(1)}, \mathbf{e}^{(2)}$ and a linear combination of $\mathbf{e}^{(13)}$ and $\mathbf{e}^{(20)}$. Thus only three coefficients are necessary.

For orthorhombic, hexagonal and tetragonal symmetry, the number of base tensors in the decomposition is nine, five and six, respectively, with the chosen coordinate system.

For trigonal symmetry, the number of base tensors is six when the coordinate system is such that $c_{14} = c_{24} = c_{56} = 0$. When, instead, $c_{15} = c_{25} = c_{46} = 0$, seven base tensors are needed. However, the contribution from $\mathbf{e}^{(16)}$ and $\mathbf{e}^{(19)}$ can be replaced by a contribution from a base tensor which is a linear combination of the two.

The decomposition shown in the tables indicates the same pattern of subsystems of symmetry as displayed in Fig. 3.1.

Also, Table 3.3 shows the decomposition into base tensors for different symmetry classes. For monoclinic, tetragonal, trigonal and hexagonal symmetry, decomposition corresponding to three different orientations of the symmetry coordinate system is shown. The decomposition generally depends on the coordinate system. Also the number of different base tensors in the decomposition depends on the coordinate system. For orthorhombic and cubic symmetry, as for isotropy, the decomposition is the same for all symmetry coordinate systems.

3.6 Quantitative measure of deviation from symmetry

The elastic tensor is generally given by 21 elastic constants different from zero. Isotropic tensors have two independent constants in all coordinate systems. If the medium has some kind of symmetry, the number of elastic constants is still 21 if the coordinate system is not a symmetry coordinate system for the medium. Even if the coordinate system is "as close as possible" to the symmetry axes of the medium, there are still 21 constants because of errors in the measurements. Also, since the real world does not possess ideal symmetry, a recorded elastic tensor has generally 21 elastic constants. If however, the coordinate system is close to the symmetry axes of the medium, the deviation from symmetry introduced in the following is small. Thus, a small deviation indicates that the medium has approximately the kind of symmetry investigated and that the coordinate axes are symmetry axes of the medium. The value of the deviation has to be compared with the norm of the tensor. If the deviation is large, there are three possibilities. Either the medium is far from the investigated symmetry, the symmetry axes are far from the coordinate axes, or a combination.

The deviation from symmetry for a tensor E_{ijkl} can be given by the following definition: the deviation is relative to a tensor of a symmetry class which is referred to a symmetry coordinate system.

We define a quantity $\Delta\mathbf{E}$ as

$$\Delta\mathbf{E} = \sum_i a_i \mathbf{e}^{(i)}. \tag{3.33}$$

The summation is taken over those i which correspond to vanishing coefficients in the decomposition of the symmetry class under consideration.

The norm of $\Delta\mathbf{E}$ is $\sqrt{\Delta E_{ijkl}\Delta E_{ijkl}}$ and the deviation is defined as:

$$\text{Deviation} = \frac{\sqrt{\Delta E_{ijkl}\Delta E_{ijkl}}}{\sqrt{E_{ijkl}E_{ijkl}}}. \tag{3.34}$$

3.7 Conclusion

An experimentally determined elastic tensor generally has 21 elastic constants different from zero. If the medium has a kind of symmetry (higher than triclinic), the number of elastic constants is still 21 if the coordinate system is not a symmetry coordinate system for the medium. Even if the coordinate system is "as close as possible" to the symmetry axes of the medium, there are still 21 constants because of errors in the measurements. If the coordinate system is close to the symmetry of the medium, the deviation from symmetry is small. To handle quantitative measures of deviation, a set of base tensors and a metric is presented. The elastic tensor is decomposed into 21 orthonormal base tensors in a 21-dimensional vector space. The base tensors are derived from harmonic tensors.

By means of the metric, deviation from spesific symmetry classes is defined. For the different symmetry classes, monoclinic, orthorhombic etc., a decomposition of the elastic tensor into the 21 base tensors is presented.

The number of base tensors needed in the decomposition is in many cases equal to the number of independent elastic constants in the elastic tensor. The decomposition however depends on the orientation of the coordinate system. The 21 base tensors form an orthonormal base of a vector space. Thus there exists a number of linear combinations of base tensors equal to the number of independent elastic constants in the elastic tensor under consideration.

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Appendix

21 orthonormal elastic base tensors in matrix representation

$$e^{(1)} = \frac{1}{\sqrt{45}} \begin{pmatrix} 3 & 1 & 1 & 0 & 0 & 0 \\ & 3 & 1 & 0 & 0 & 0 \\ & & 3 & 0 & 0 & 0 \\ & & & 1 & 0 & 0 \\ & & & & 1 & 0 \\ & & & & & 1 \end{pmatrix} \qquad \text{Isotropic symmetry}$$

$$e^{(2)} = \frac{1}{3} \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ & 0 & 1 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & -0.5 & 0 & 0 \\ & & & & -0.5 & 0 \\ & & & & & -0.5 \end{pmatrix} \qquad \text{Isotropic symmetry}$$

$$e^{(3)} = \frac{1}{\sqrt{252}} \begin{pmatrix} 6 & 2 & -1 & 0 & 0 & 0 \\ & 6 & -1 & 0 & 0 & 0 \\ & & -12 & 0 & 0 & 0 \\ & & & -1 & 0 & 0 \\ & & & & -1 & 0 \\ & & & & & 2 \end{pmatrix} \quad \text{Hexagonal symmetry}$$

$$e^{(4)} = \frac{1}{3\sqrt{2}} \begin{pmatrix} 0 & 2 & -1 & 0 & 0 & 0 \\ & 0 & -1 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0.5 & 0 & 0 \\ & & & & 0.5 & 0 \\ & & & & & -1 \end{pmatrix} \quad \text{Hexagonal symmetry}$$

$$e^{(5)} = \frac{1}{2\sqrt{21}} \begin{pmatrix} 0 & 0 & 0 & 0 & 3 & 0 \\ & 0 & 0 & 0 & 1 & 0 \\ & & 0 & 0 & 3 & 0 \\ & & & 0 & 0 & 1 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(6)} = \frac{1}{2\sqrt{6}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 1 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & -0.5 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(7)} = \frac{1}{2\sqrt{21}} \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ & 0 & 0 & 3 & 0 & 0 \\ & & 0 & 3 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & 1 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(8)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ & 0 & 0 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & -0.5 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(9)} = \frac{1}{2\sqrt{21}} \begin{pmatrix} 6 & 0 & 1 & 0 & 0 & 0 \\ & -6 & -1 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & -1 & 0 & 0 \\ & & & & 1 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Orthorhombic symmetry}$$

$$e^{(10)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ & 0 & -1 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0.5 & 0 & 0 \\ & & & & -0.5 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Orthorhombic symmetry}$$

$$e^{(11)} = \frac{1}{2\sqrt{21}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 3 \\ & 0 & 0 & 0 & 0 & 3 \\ & & 0 & 0 & 0 & 1 \\ & & & 0 & 1 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(12)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 1 \\ & & & 0 & -0.5 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(13)} = \frac{1}{2\sqrt{70}} \begin{pmatrix} 3 & 1 & -4 & 0 & 0 & 0 \\ & 3 & -4 & 0 & 0 & 0 \\ & & 8 & 0 & 0 & 0 \\ & & & -4 & 0 & 0 \\ & & & & -4 & 0 \\ & & & & & 1 \end{pmatrix} \quad \text{Hexagonal symmetry}$$

$$e^{(14)} = \frac{1}{4\sqrt{7}} \begin{pmatrix} 0 & 0 & 0 & 0 & 3 & 0 \\ & 0 & 0 & 0 & 1 & 0 \\ & & 0 & 0 & -4 & 0 \\ & & & 0 & 0 & 1 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(15)} = \frac{1}{4\sqrt{7}} \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ & 0 & 0 & 3 & 0 & 0 \\ & & 0 & -4 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & 1 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(16)} = \frac{1}{\sqrt{14}} \begin{pmatrix} 1 & 0 & -1 & 1 & 0 & 0 \\ & -1 & 1 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 1 & 0 & 0 \\ & & & & -1 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(17)} = \frac{1}{2\sqrt{14}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ & 0 & 0 & 0 & 0 & 1 \\ & & 0 & 0 & 0 & -2 \\ & & & 0 & -2 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(18)} = \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ & 0 & 0 & 0 & -1 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & -1 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \quad \text{Hexagonal symmetry}$$

$$e^{(19)} = \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 \\ & 0 & 0 & 1 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & -1 \\ & & & & & 0 \end{pmatrix} \quad \text{Monoclinic symmetry}$$

$$e^{(20)} = \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ & 1 & 0 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & 0 \\ & & & & & -1 \end{pmatrix} \quad \text{Tetragonal symmetry}$$

$$e^{(21)} = \frac{1}{2\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ & 0 & 0 & 1 & 0 & -1 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix}$$

Tetragonal symmetry

Chapter 4

Classification of symmetry by means of Maxwell multipoles

Abstract

It is well known that elastic tensors are classified according to higher symmetry as monoclinic, orthorhombic etc. A classification into these classes by means of bouquets of space directions, called Maxwell multipoles, is given, and explicit expressions for the magnitudes of the directions are developed. The analysis is based on harmonic decomposition of the hierarchically symmetric tensor presented in Backus (**1**), and further developed in Ch. 2. Hierarchically symmetric tensors are defined as fourth rank tensors in three dimensions, satisfying the symmetry conditions $E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}$. Software is developed to calculate the bouquets of space directions, and MATHEMATICA is used for displaying the results. As an example, multipoles are calculated for a specific tensor of monoclinic symmetry.

4.1 Introduction

In an anisotropic material the elastic tensor generally has 21 non-vanishing constants. Decomposition of the elastic tensor in harmonic tensors is useful in determining the symmetry properties of elastic media. Different ways for such decomposition have been specified; see (**1**), (**3**) and (**4**). The present approach is based on the harmonic decomposition given by Backus (**1**) and in Ch.2.

An approach related to spectral decomposition is suggested by Sutcliffe (**5**), where the elastic tensor **C** is regarded as a symmetric linear transformation on the space

This chapter has been accepted for publication in Q. Jl. Mech. appl. Math. as:
Reidar Baerheim, Classification of symmetry by means of Maxwell multipoles

of symmetric second rank tensors. $\mathbf{C}$ is represented as a second rank tensor in six dimensions. The spectral decomposition of $\mathbf{C}$ is given by

$$\mathbf{C} = \lambda_k(\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)}), \quad \text{summation over } k,\ k = 1, \ldots, 6, \tag{4.1}$$

where λ_k is the eigenvalue of $\mathbf{C}$ corresponding to the eigenvector $\mathbf{n}^{(k)}$. The components of the tensor product $\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)}$ (for a specific k) relative to a specific basis are then given by the components of $\mathbf{n}^{(k)}$:

$$(\mathbf{n}^{(k)} \otimes \mathbf{n}^{(k)})_{ij} = n_i^{(k)} n_j^{(k)}, \quad i = 1, \ldots, 6,\ j = 1, \ldots, 6, \text{ no summation over } k.$$

An eigenvector of the elastic tensor in six dimensions, represented as a second rank tensor in three dimensions, is called an eigentensor. The six normalized eigentensors and the six eigenvalues (eigenstiffnesses) completely define the elastic tensor. Eigentensors and eigenstiffnesses are treated by Helbig (**6**, ch.11) as well, where the theory is mainly based on papers by Kelvin (**7**, **8**), Pipkin (**9**), Rychlewski (**10**) and Mehrabadi and Cowin (**11**).

In Backus's decomposition, the elastic tensor is decomposed into five harmonic tensors expressed explicitly by the elastic stiffnesses (see the definition of harmonic tensor below). Sutcliffe (**5**) does not give explicitly the general expression of the six eigentensors and the eigenvalues in (4.1).

In the further development an elastic tensor E is defined as a positive definite tensor of rank four and dimension three with the symmetry properties

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}. \tag{4.2}$$

A tensor is said to be positive definite if $\epsilon_{ij}\epsilon_{kl}E_{ijkl} > 0$ for all ϵ_{ij}. A tensor defined by (4.2) is here called hierarchically symmetric.

Harmonic tensors are defined as totally symmetric and traceless tensors. In a totally symmetric tensor all tensor components with a specific set of indices are equal, regardless of the permutation of the indices. A tensor is traceless when the contraction of all pairs of two indices is zero. Harmonic tensors of a specific rank thus define a subset of hierarchically symmetric tensors.

Generally, each hierarchically symmetric tensor generates a homogeneous polynomial in three variables of degree four. The polynomial has at most 15 independent terms.

According to Backus (**1**) (see also Ch. 2), the following strategy is followed in the development of a geometrical representation of the hierarchically symmetric tensor by means of harmonic decomposition:

1. A hierarchically symmetric tensor can be separated into a sum of a totally symmetric part (at most 15 independent constants), and the remainder, a non-totally symmetric part (at most six independent constants).

2. Each of the two parts is isomorphic to a homogeneous polynomial in three variables of degree four and two, respectively. The totally symmetric part

is isomorphic to the homogeneous polynomial generated by the hierarchically symmetric tensor.

3. A homogeneous polynomial of degree $2m$ can be uniquely decomposed into harmonic polynomials of degree $2m, 2(m-1), \ldots$. A hierarchically symmetric tensor is thus isomorphic to five harmonic polynomials. A harmonic polynomial of degree $2m$ is a member of the vector space of solid spherical harmonics of degree $2m$.

4. Harmonic polynomials are isomorphic to Maxwell multipoles (double vectors) and provide a coordinate-free representation of the above five parts of the hierarchically symmetric tensor.

5. The components of Maxwell multipoles are determined from the harmonic polynomials in the following way:

   (a) A homogeneous polynomial in three variables of degree q is mapped on a homogeneous polynomial of degree $2q$ with complex coefficients in two variables.

   (b) A homogeneous polynomial of degree $2q$ in two variables is mapped on an inhomogeneous polynomial of degree $2q$ in one variable. The roots of these polynomials are directly related to the components of the Maxwell multipoles.

   Thus there is a unique decomposition of a hierarchically symmetric tensor into harmonic tensors of rank four, two and zero.

According to Sylvester's theorem, each harmonic polynomial corresponds to a set of vectors, represented as unit vectors and magnitude. The vectors are uniquely determined except for the sign. For a proof, see (**1**). Thus a vector and its negative define a line, which we call a direction. The bouquet of directions associated to a harmonic polynomial determine a Maxwell multipole (see also (**12**)). There are a few minor misprints in Backus's proof which are tacitly corrected here. Guidelines for determining those directions are contained in the proof. In the present paper it is shown how to use the guidelines for finding explicit expressions for the space directions. In addition the magnitude is calculated. A classification of the different symmetry systems by means of Maxwell multipoles is given. The calculation of multipoles is implemented on the software package developed by Professor Klaus Helbig. The bouquets of directions for given elastic tensors are given. It is illustrated how this can be used to classify symmetry when the tensor is related to a coordinate system which is not the symmetry coordinate system.

4.2 Sylvester's theorem

Any real homogeneous polynomial $P^{(q)}(\mathbf{r})$ of degree q and dimension three can be expressed in the following way (**1**):

$$P^{(q)}(\mathbf{r}) = A\prod_{\nu=1}^{q}(\hat{\mathbf{a}}_\nu \cdot \mathbf{r}) + r^2 P^{(q-2)}(\mathbf{r}), \tag{4.3}$$

where $\hat{\mathbf{a}}_\nu$ are unit vectors defined by $P^{(q)}(\mathbf{r})$ and $\hat{\mathbf{a}}_\nu \cdot \mathbf{r}$ is a scalar product. The polynomial $P^{(q-2)}(\mathbf{r})$ and the scalar A are uniquely determined by $P^{(q)}(\mathbf{r})$, and the set of directions $\hat{\mathbf{a}}_\nu$ is uniquely determined to within sign changes of an even number of $\hat{\mathbf{a}}_\nu$. This means that to each $\hat{\mathbf{a}}_\nu$, the opposite vector is also a solution. Together the two unit vectors define a space direction along a line.

To each harmonic tensor corresponds uniquely a harmonic polynomial $H^{(q)}(\mathbf{r})$. Sylvester's theorem applied to harmonic polynomials of degree four, for example, gives

$$H^{(4)}(\mathbf{r}) = A\prod_{\nu=1}^{4}(\hat{\mathbf{a}}_\nu \cdot \mathbf{r}) + r^2 P^{(2)}(\mathbf{r}). \tag{4.4}$$

This means that to each harmonic polynomial of fourth degree, corresponds a set of four space directions defined above. Therefore, to each harmonic tensor of rank four corresponds a bouquet of four space directions defined above.

In the following a method of finding the unit vectors $\hat{\mathbf{a}}_\nu$ is presented. This is based on the theory presented by Backus (**1**). In addition, explicit expressions for the magnitude A are given.

We start by defining a homomorphism Ψ from $C_3^\infty(x,y,z)$ to $C_2^{2\infty}(\xi,\eta)$ where $C_3^\infty(x,y,z)$ is the ring of all polynomials in the three indeterminates x, y and z and $C_2^{2\infty}(\xi,\eta)$ is the ring of all even polynomials in the two indeterminates ξ and η. (In this general development, the rings contain not only homogeneous polynomials.) All polynomials are allowed to have complex coefficients. A ring is a set of elements with two binary operations. For polynomial rings, the operations are addition and multiplication. The two operations (in each of the rings) satisfy the fundamental laws of elementary algebra. Both operations are for example commutative since multiplication of two polynomials is commutative (see (**13**) or (**14**) for further algebraic theory).

Generally, a homomorphism Φ from ring1 to ring2 satisfies

$$\Phi(fg) = \Phi(f)\cdot\Phi(g) \quad \text{and} \quad \Phi(f+g) = \Phi(f) + \Phi(g),$$

where f and g are elements in ring1. In our case, f and g are polynomials in $C_3^\infty(x,y,z)$.

The homomorphism Ψ is defined by

$$\Psi(a) = a, \quad a \text{ is a complex constant}, \quad \Psi(x) = \xi^2 - \eta^2,$$

$$\Psi(y) = -i(\xi^2 + \eta^2), \quad \Psi(z) = 2\xi\eta, \tag{4.5}$$

where i is the imaginary unit.

Let us denote the homogeneous polynomials in $C_3^{\infty}(x, y, z)$ by $P^{(q)}$ and the polynomials in $C_2^{2\infty}(\xi, \eta)$ by $p^{(2q)}$; q and $2q$ are the degrees of the polynomials in the two rings respectively.

Example 1

Let us consider the Ψ-mapping of a general homogeneous polynomial of second degree in three indeterminates with real coefficients. This example illustrates some properties of Ψ, when applied to homogeneous polynomials:

$$P^{(2)}(x, y, z) = ax^2 + bxy + cxz + dy^2 + eyz + fz^2,$$

$$\Psi(P^{(2)}(x, y, z)) = \Psi(ax^2) + \Psi(bxy) + \Psi(cxz) + \Psi(dy^2) + \Psi(eyz) + \Psi(fz^2).$$

Since, for example,

$$\Psi(ax^2) = \Psi(a) \cdot \Psi(x^2) = a(\xi^2 - \eta^2)^2$$

and

$$\Psi(bxy) = \Psi(b) \cdot \Psi(x) \cdot \Psi(y) = b(\xi^2 - \eta^2)(-i(\xi^2 + \eta^2)),$$

we get

$$\Psi(P^{(2)}(x, y, z)) = a(\xi^2 - \eta^2)^2 + b(\xi^2 - \eta^2)(-i(\xi^2 + \eta^2)) + c(\xi^2 - \eta^2)2\xi\eta$$
$$+d(-i(\xi^2 + \eta^2))^2 + e(-i(\xi^2 + \eta^2))2\xi\eta + 4f\xi^2\eta^2.$$

By using the notation $\Psi(P^{(2)}(x, y, z)) = p^{(4)}(\xi, \eta)$, we further have

$$p^{(4)}(\xi, \eta) = a(\xi^4 - 2\xi^2\eta^2 + \eta^4) - ib(\xi^4 - \eta^4) + 2c(\xi^3\eta - \xi\eta^3)$$
$$-d(\xi^4 + 2\xi^2\eta^2 + \eta^4) - i2e(\xi^3\eta + \xi\eta^3) + 4f\xi^2\eta^2. \tag{4.6}$$

After rearranging, (4.6) becomes

$$p^{(4)}(\xi, \eta) = \xi^4(a - d - ib) + \xi^3\eta(2c - i2e)$$
$$+\xi^2\eta^2(-2a - 2d + 4f) + \xi\eta^3(-2c - i2e) + \eta^4(a - d + ib),$$

which is a homogeneous polynomial of fourth degree in ξ and η with complex coefficients.

Generally we have

$$p^{(2q)}(\xi, \eta) = \sum_{\nu=0}^{2q} C_\nu \xi^{2q-\nu}\eta^\nu. \tag{4.7}$$

Dividing this expression by η^{2q}, and then letting $t = \xi/\eta$, gives

$$p^{(2q)}(t, 1) = \sum_{\nu=0}^{2q} C_\nu t^{2q-\nu}, \tag{4.8}$$

which is a polynomial of degree $2q$ in one indeterminate t. The complex conjugate of (4.7) is

$$p^{(2q)*}(\xi,\eta) = \sum_{\nu=0}^{2q} C_\nu^* \xi^{2q-\nu}\eta^\nu.$$

In the further development we also need an expression for $p^{(2q)*}(-\eta,\xi)$.

Example 1, continued

From (4.6) in our example, the complex conjugate of $p^{(4)}(-\eta,\xi)$ is given by

$$\begin{aligned} p^{(4)*}(-\eta,\xi) &= a(\eta^4 - 2\xi^2\eta^2 + \xi^4) - ib(\xi^4 - \eta^4) + 2c(\xi^3\eta - \xi\eta^3) \\ &\quad -d(\eta^4 + 2\xi^2\eta^2 + \xi^4) - i2e(\xi^3\eta + \xi\eta^3) + 4f\xi^2\eta^2. \end{aligned} \tag{4.9}$$

Comparing (4.6) and (4.9) we notice that $p^{(4)*}(-\eta,\xi) = p^{(4)}(\xi,\eta)$.

Generally we have $p^{(2q)*}(-\eta,\xi) = (-1)^q p^{(2q)}(\xi,\eta)$, and therefore

$$p^{(2q)*}(-1,t) = (-1)^q p^{(2q)}(t,1). \tag{4.10}$$

Suppose z is a root of $p^{(2q)}(t,1)$, that is

$$p^{(2q)}(z,1) = 0. \tag{4.11}$$

Further, from (4.10) it follows that $p^{(2q)*}(-1,z) = 0$. Therefore also

$$p^{(2q)}(-1,z^*) = 0 \tag{4.12}$$

by complex conjugating. We will now find an expression for $p^{(2q)}(-1,z^*)$. From (4.7) we have

$$\begin{aligned} p^{(2q)}(-1,z^*) &= C_0(-1)^{2q} + C_1(-1)^{2q-1}z^* + C_2(-1)^{2q-2}z^{*2} + \cdots + C_{2q}z^{*2q} \\ &= C_0 - C_1 z^* + C_2 z^{*2} - \cdots + C_{2q}z^{*2q}. \end{aligned}$$

Divide this equation by z^{*2q} to get

$$(p^{(2q)}(-1,z^*))/z^{*2q} = C_0(1/z^*)^{2q} - C_1(1/z^*)^{2q-1} + \cdots + C_{2q},$$

which is equal to $p^{(2q)}(-1/z^*,1)$. This is seen by using (4.8), for instance. We have then shown that

$$p^{(2q)}(-1,z^*) = z^{*2q}p^{(2q)}(-1/z^*,1). \tag{4.13}$$

This means that if $p^{(2q)}(-1,z^*) = 0$, then $p^{(2q)}(-1/z^*,1) = 0$. Thus from (4.11), (4.12) and (4.13): *if z is a root in $p^{(2q)}(t,1)$, then $-1/z^*$ is a root also.* Therefore, if $t - z$ is a factor of $p(t,1)$, $t + 1/z^*$ is a factor as well (at this point Backus (**1**) has a misprint). If $r\xi + s\eta$ is a factor of $p(\xi,\eta)$ then $rt + s$ is a factor of $p(t,1)$

where $t = \xi/\eta$. Thus $t + s/r = t - z$ is a factor of $p(t,1)$ where $z = -s/r$. Thus $t+1/z^* = t-(r/s)^*$ is a factor. Further, if $t-(r/s)^*$ is a factor then s^*t-r^* is a factor which implies that $s^*\xi/\eta - r^*$ is a factor and so $s^*\xi - r^*\eta$ is a factor. Thus $r\xi + s\eta$ and $s^*\xi - r^*\eta$ are factors of $p^{(2q)}(\xi,\eta)$. Since $p^{(2q)}(\xi,\eta)$ is a homogeneous polynomial of degree $2q$, there are $2q$ roots. Thus $p^{(2q)}(\xi,\eta)$ is the product of q factors of the form $(r_\nu\xi + s_\nu\eta)(s_\nu^*\xi - r_\nu^*\eta)$, that is

$$p^{(2q)}(\xi,\eta) = \prod_{\nu=1}^{q}(r_\nu\xi + s_\nu\eta)(s_\nu^*\xi - r_\nu^*\eta). \tag{4.14}$$

We have the following identity:

$$(r\xi + s\eta)(s^*\xi - r^*\eta) = \tfrac{1}{2}(rs^* + r^*s)(\xi^2 - \eta^2)$$
$$+\tfrac{1}{2}i(rs^* - r^*s)(-i(\xi^2 + \eta^2)) + \tfrac{1}{2}(ss^* - rr^*)2\xi\eta. \tag{4.15}$$

Notice that the right side of this identity has the form

$$a\Psi(x) + b\Psi(y) + c\Psi(z),$$

where

$$a = \tfrac{1}{2}(rs^* + r^*s), \quad b = \tfrac{1}{2}i(rs^* - r^*s) \quad \text{and} \quad c = \tfrac{1}{2}(ss^* - rr^*). \tag{4.16}$$

Thus $p^{(2q)}(\xi,\eta)$ has the form $\Psi(Q^{(q)})$, where

$$Q^{(q)} = \prod_{\nu=1}^{q}(a_\nu x + b_\nu y + c_\nu z).$$

Define $V^{(q)}$ in such a way that $\Psi(V^{(q)}) \equiv 0$. Then if $Q^{(q)} = P^{(q)} - V^{(q)}$ we have $\Psi(Q^{(q)}) = \Psi(P^{(q)})$. Thus

$$P^{(q)} = \prod_{\nu=1}^{q}(a_\nu x + b_\nu y + c_\nu z) + V^{(q)}. \tag{4.17}$$

We will now express a, b and c by means of the real and imaginary parts of the roots of $p(t,1)$. Let $z = k + il$ be a root of $p(t,1)$. For example, from (4.16) we have $a = \frac{1}{2}(rs^* + r^*s) = \frac{1}{2}(-z^* - z)rr^* = -krr^*$. We calculate b and c similarly, giving

$$a = -krr^*, \quad b = -lrr^* \quad \text{and} \quad c = \tfrac{1}{2}(k^2 + l^2 - 1)rr^*. \tag{4.18}$$

4.3 Maxwell multipoles for harmonic tensors

Each hierarchically symmetric tensor is related to one harmonic tensor of rank four, two harmonic tensors of rank two, and two scalars (1). To find the multipoles, we first transform each harmonic polynomial of degree q to a polynomial in one indeterminate of degree $2q$. Once the roots of the polynomial are determined, the bouquet of space directions in the multipole is known.

Equation (2.29) Ch. 2 gives the harmonic tensor of rank four expressed by means of the hierarchically symmetric tensor:

$$H_{ijkl} = S_{ijkl} - Q_{ij}\delta_{kl} - Q_{kl}\delta_{ij} - Q_{ik}\delta_{jl} - Q_{jl}\delta_{ik} - Q_{il}\delta_{jk} - Q_{jk}\delta_{il} + \tfrac{1}{5}Q_{mm}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{4.19}$$

where S_{ijkl} is the totally symmetric part of the tensor, and Q is defined by

$$Q_{ij} = \tfrac{1}{21}(C_{ij} + 2V_{ij}). \tag{4.20}$$

Here C and V are the dilatational modulus tensor and Voigt tensor respectively, and are given by

$$C_{ij} = E_{ijkk} = \begin{pmatrix} c_{11}+c_{12}+c_{13} & c_{16}+c_{26}+c_{36} & c_{15}+c_{25}+c_{35} \\ & c_{12}+c_{22}+c_{23} & c_{14}+c_{24}+c_{34} \\ & & c_{13}+c_{23}+c_{33} \end{pmatrix}, \tag{4.21}$$

$$V_{ij} = E_{ikkj} = \begin{pmatrix} c_{11}+c_{55}+c_{66} & c_{16}+c_{26}+c_{45} & c_{15}+c_{46}+c_{35} \\ & c_{22}+c_{44}+c_{66} & c_{24}+c_{34}+c_{56} \\ & & c_{33}+c_{44}+c_{55} \end{pmatrix}, \tag{4.22}$$

where c_{ij} are the elastic stiffnesses in two-index notation, see (**3**, **15**).

The deviatoric part of a tensor T_{ij} is defined by $\hat{T}_{ij} = T_{ij} - \frac{1}{3}T_{ii}\delta_{ij}$. Note that $\hat{C}_{ij}$ and $\hat{V}_{ij}$ are equal to C_{ij} and V_{ij}, respectively, except for the diagonal elements which are given as follows:

$$\begin{aligned} \hat{C}_{11} &= \tfrac{2}{3}(c_{11} - c_{23}) - \tfrac{1}{3}(c_{22} + c_{33} - c_{12} - c_{13}), \\ \hat{C}_{22} &= \tfrac{2}{3}(c_{22} - c_{13}) - \tfrac{1}{3}(c_{11} + c_{33} - c_{12} - c_{23}), \\ \hat{C}_{33} &= \tfrac{2}{3}(c_{33} - c_{12}) - \tfrac{1}{3}(c_{11} + c_{22} - c_{13} - c_{23}), \end{aligned} \tag{4.23}$$

and

$$\begin{aligned} \hat{V}_{11} &= \tfrac{2}{3}(c_{11} - c_{44}) - \tfrac{1}{3}(c_{22} + c_{33} - c_{55} - c_{66}), \\ \hat{V}_{22} &= \tfrac{2}{3}(c_{22} - c_{55}) - \tfrac{1}{3}(c_{11} + c_{33} - c_{44} - c_{66}), \\ \hat{V}_{33} &= \tfrac{2}{3}(c_{33} - c_{66}) - \tfrac{1}{3}(c_{11} + c_{22} - c_{44} - c_{55}). \end{aligned} \tag{4.24}$$

Since H_{ijkl} is harmonic and thus totally symmetric, the tensor has at most 15 different components. From (4.19), the components of H_{ijkl} are

$$\begin{aligned} H_{1111} &= E_{1111} - 6Q_{11} + \tfrac{3}{5}Q_{mm}, & H_{1112} &= E_{1112} - 3Q_{12}, \\ H_{1122} &= S_{1122} - Q_{11} - Q_{22} + \tfrac{1}{5}Q_{mm}, & H_{1113} &= E_{1113} - 3Q_{13}, \end{aligned}$$

$$\begin{aligned}
H_{1133} &= S_{1133} - Q_{11} - Q_{33} + \tfrac{1}{5}Q_{mm}, & H_{1123} &= S_{1123} - Q_{23},\\
H_{1222} &= E_{1222} - 3Q_{12}, & H_{1223} &= S_{1223} - Q_{13},\\
H_{1233} &= S_{1233} - Q_{12}, & H_{1333} &= E_{1333} - 3Q_{13},\\
H_{2222} &= E_{2222} - 6Q_{22} + \tfrac{3}{5}Q_{mm}, & H_{2223} &= E_{2223} - 3Q_{23},\\
H_{2233} &= S_{2233} - Q_{22} - Q_{33} + \tfrac{1}{5}Q_{mm}, & H_{2333} &= E_{2333} - 3Q_{23},\\
H_{3333} &= E_{3333} - 6Q_{33} + \tfrac{3}{5}Q_{mm},
\end{aligned} \tag{4.25}$$

where E_{ijkl} is the hierarchically symmetric tensor. Components of S_{ijkl} are replaced by corresponding components of the hierarchically symmetric tensor where there is equality between the two.

The homogeneous polynomial generated by the harmonic tensor can be transformed to a polynomial in one variable after application of Ψ, defined by (4.5). Transformation of the fourth degree homogeneous polynomial $P^{(4)}$ gives an eighth degree polynomial in t. The fourth degree polynomial generated by a harmonic tensor of rank 4 is given in Ch. 2 as

$$\begin{gathered}
P^{(4)}(x,y,z) = H_{1111}x^4 + 4H_{1112}x^3y + 4H_{1113}x^3z\\
+6H_{1122}x^2y^2 + 12H_{1123}x^2yz + 6H_{1133}x^2z^2 + 4H_{1222}xy^3\\
+12H_{1223}xy^2z + 12H_{1233}xyz^2 + 4H_{1333}xz^3 + H_{2222}y^4\\
+4H_{2223}y^3z + 6H_{2233}y^2z^2 + 4H_{2333}yz^3 + H_{3333}z^4.
\end{gathered}$$

The derivation of the eighth degree polynomial in t from the fourth degree harmonic homogeneous polynomial $P^{(4)}(x,y,z)$ is performed by the Ψ-mapping in (4.5). By applying Ψ, and replacing ξ and η by t and 1, respectively, the above expression for $P^{(4)}(x,y,z)$ is transformed to the following eighth degree polynomial in t (see the transformation from (4.7) to (4.8)):

$$\begin{gathered}
p^{(8)}(t) = (H_{1111} - 6H_{1122} + H_{2222} + 4i(-H_{1112} + H_{1222}))t^8+\\
8(H_{1113} - 3H_{1223} + i(-3H_{1123} + H_{2223}))t^7+\\
4(-H_{1111} + 6H_{1133} + H_{2222} - 6H_{2233} + 2i(H_{1112} + H_{1222} - 6H_{1233}))t^6+\\
8(-3H_{1113} - 3H_{1223} + 4H_{1333} + i(3H_{1123} + 3H_{2223} - 4H_{2333}))t^5+\\
2(3H_{1111} + 6H_{1122} - 24H_{1133} + 3H_{2222} - 24H_{2233} + 8H_{3333})t^4+\\
8(3H_{1113} + 3H_{1223} - 4H_{1333} + i(3H_{1123} + 3H_{2223} - 4H_{3332}))t^3+\\
4(-H_{1111} + 6H_{1133} + H_{2222} - 6H_{2233} + 2i(-H_{1112} - H_{1222} + 6H_{1233}))t^2+\\
8(-H_{1113} + 3H_{1223} + i(-3H_{1123} + H_{2223}))t+\\
H_{1111} - 6H_{1122} + H_{2222} + 4i(H_{1112} - H_{1222})
\end{gathered} \tag{4.26}$$

which has the form

$$p^{(8)}(t) = a_8t^8 + a_7t^7 + a_6t^6 + a_5t^5 + a_4t^4 - a_5^*t^3 + a_6^*t^2 - a_7^*t + a_8^*,$$

where $*$ denotes complex conjugate.

We will now express the coefficients in the eighth degree polynomial (4.26) in terms of elastic constants. Substituting (4.25) into (4.26), using (4.20), (4.21) and (4.22), gives

$$\begin{aligned}
a_8 &= c_{11} + c_{22} - 4c_{66} - 2c_{12} + 4i(-c_{16} + c_{26}),\\
a_7 &= 8[c_{15} - c_{25} - 2c_{46} + i(-c_{14} + c_{24} - 2c_{56})],\\
a_6 &= 4[-c_{11} + c_{22} - 4c_{44} + 4c_{55} + 2c_{13} - 2c_{23} + 2i(c_{16} + c_{26} - 2c_{36} - 4c_{45})],\\
a_5 &= 8[-3c_{15} - c_{25} + 4c_{35} - 2c_{46} + i(c_{14} + 3c_{24} - 4c_{34} + 2c_{56}),\\
a_4 &= 2[3c_{11} + 3c_{22} + 8c_{33} - 16c_{44} - 16c_{55} + 4c_{66} + 2c_{12} - 8c_{13} - 8c_{23}],\\
a_3 &= -a_5^*, \qquad a_2 = a_6^*, \qquad a_1 = -a_7^*, \qquad a_0 = a_8^*.
\end{aligned} \tag{4.27}$$

The second degree polynomial generated by any specific harmonic tensor $\mathcal{H}$ of rank 2 is

$$P^{(2)}(x,y,z) = \mathcal{H}_{11}x^2 + \mathcal{H}_{22}y^2 + \mathcal{H}_{33}z^2 + 2\mathcal{H}_{12}xy + 2\mathcal{H}_{13}xz + 2\mathcal{H}_{23}yz.$$

Similarly to the derivation of (4.26), transformation of this second degree harmonic homogeneous polynomial $P^{(2)}(x,y,z)$ by Ψ, gives fourth degree polynomial in t which has the form

$$p^{(4)}(t) = a_4^{(\mathcal{H})}t^4 + a_3^{(\mathcal{H})}t^3 + a_2^{(\mathcal{H})}t^2 - a_3^{(\mathcal{H})*}t + a_4^{(\mathcal{H})*}, \tag{4.28}$$

where

$$\begin{aligned}
a_4^{(\mathcal{H})} &= \mathcal{H}_{11} - \mathcal{H}_{22} - 2i\mathcal{H}_{12}, \quad a_3^{(\mathcal{H})} = 4(\mathcal{H}_{13} - i\mathcal{H}_{23}),\\
a_2^{(\mathcal{H})} &= 2(-\mathcal{H}_{11} - \mathcal{H}_{22} + 2\mathcal{H}_{33}).
\end{aligned} \tag{4.29}$$

In the decomposition of the hierarchically symmetric tensor in harmonic tensors according to Backus, there are two second rank harmonic tensors, H_{ij} and h_{ij}. Of these H_{ij} is related to the totally symmetric part of the hierarchically symmetric tensor, and h_{ij} is related to the non-totally symmetric part. Further H_{ij} is given in Ch. 2 as

$$H_{ij} = \tfrac{1}{21}(\hat{C}_{ij} + 2\hat{V}_{ij}). \tag{4.30}$$

Substitution of (4.30) into (4.29), using (4.23) and (4.24), gives

$$\begin{aligned}
a_4^{(H)} &= \tfrac{1}{21}[3c_{11} - 3c_{22} - 2c_{44} + 2c_{55} + c_{13} - c_{23} - 2i(3c_{16} + 3c_{26} + c_{36} + 2c_{45})],\\
a_3^{(H)} &= \tfrac{4}{21}[3c_{15} + c_{25} + 3c_{35} + 2c_{46} - i(c_{14} + 3c_{24} + 3c_{34} + 2c_{56})],\\
a_2^{(H)} &= \tfrac{2}{21}[-3c_{11} - 3c_{22} + 6c_{33} + 2c_{44} + 2c_{55} - 4c_{66} - 2c_{12} + c_{13} + c_{23}],
\end{aligned} \tag{4.31}$$

which are the coefficients in the polynomial (4.28) corresponding to the second rank tensor associated to the totally symmetric part of the hierarchically symmetric tensor.

We will now find the magnitude A in (4.3) for the harmonic tensors. For reasons of instruction and simplicity, the magnitude A corresponding to a second rank tensor is calculated first. The magnitude corresponding to a fourth rank tensor is calculated later. From (4.17) and the property of $V^{(q)}$ we have

$$p^{(2q)} = \Psi(P^{(q)}) = \Psi(\prod_{\nu=1}^{q}(a_\nu x + b_\nu y + c_\nu z) + V^{(q)}) = \Psi(\prod_{\nu=1}^{q}(a_\nu x + b_\nu y + c_\nu z)).$$

For $q = 2$, we have from (4.14), (4.15) and (4.18)

$$\begin{aligned} p^{(4)} &= \prod_{\nu=1}^{2}(r_\nu \xi + s_\nu \eta)(s_\nu^* \xi - r_\nu^* \eta) \\ &= [-k_1 r_1 r_1^*(\xi^2 - \eta^2) + l_1 r_1 r_1^* i(\xi^2 + \eta^2) + \tfrac{1}{2}(k_1^2 + l_1^2 - 1) r_1 r_1^*(2\xi\eta)] \\ &\times[-k_2 r_2 r_2^*(\xi^2 - \eta^2) + l_2 r_2 r_2^* i(\xi^2 + \eta^2) + \tfrac{1}{2}(k_2^2 + l_2^2 - 1) r_2 r_2^*(2\xi\eta)]. \end{aligned} \tag{4.32}$$

With the following substitutions and notation:

$$\xi = t, \quad \eta = 1 \quad \text{and} \quad M = r_1 r_1^* r_2 r_2^*, \tag{4.33}$$

we have, after rearranging, a fourth degree polynomial in t:

$$\begin{aligned} p^{(4)}(t) &= M[k_1k_2 - l_1l_2 - i(k_1l_2 + l_1k_2)]t^4 \\ &+M[-(k_1^2 + l_1^2 - 1)k_2 - k_1(k_2^2 + l_2^2 - 1) + i((k_1^2 + l_1^2 - 1)l_2 + l_1(k_2^2 + l_2^2 - 1))]t^3 \\ &+M[-2k_1k_2 - 2l_1l_2 + (k_1^2 + l_1^2 - 1)(k_2^2 + l_2^2 - 1)]t^2 \\ &+M[(k_1^2 + l_1^2 - 1)k_2 + k_1(k_2^2 + l_2^2 - 1) + i((k_1^2 + l_1^2 - 1)l_2 + l_1(k_2^2 + l_2^2 - 1))]t \\ &+M[k_1k_2 - l_1l_2 + i(k_1l_2 + l_1k_2),] \end{aligned} \tag{4.34}$$

which again shows the form given in (4.28).

Let us consider the second rank harmonic tensor associated to the totally symmetric part of the hierarchically symmetric tensor, and compare (4.34) with (4.31) in order to express M in terms of elastic constants. Combining the two complex expressions (4.34) and (4.31) for the coefficients in $p^{(4)}(t)$, and separating real and imaginary parts, we have the following five equations

$$\begin{aligned} M(k_1k_2 - l_1l_2) &= \tfrac{1}{21}(3c_{11} - 3c_{22} - 2c_{44} + 2c_{55} + c_{13} - c_{23}) \quad &\text{I} \\ M(k_1l_2 + l_1k_2) &= \tfrac{2}{21}(3c_{16} + 3c_{26} + c_{36} + 2c_{45}) \quad &\text{II} \\ M[(k_1^2 + l_1^2 - 1)k_2 + k_1(k_2^2 + l_2^2 - 1)] &= -\tfrac{4}{21}(3c_{15} + c_{25} + 3c_{35} + 2c_{46}) \quad &\text{III} \\ M[(k_1^2 + l_1^2 - 1)l_2 + l_1(k_2^2 + l_2^2 - 1)] &= -\tfrac{4}{21}(c_{14} + 3c_{24} + 3c_{34} + 2c_{56}) \quad &\text{IV} \\ M[-2k_1k_2 - 2l_1l_2 + (k_1^2 + l_1^2 - 1)(k_2^2 + l_2^2 - 1)]& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (4.35) \\ = \tfrac{2}{21}(-3c_{11} - 3c_{22} + 6c_{33} + 2c_{44} &+ 2c_{55} - 4c_{66} - 2c_{12} + c_{13} + c_{23}) \quad &\text{V} \end{aligned}$$

to determine M, k_1, k_2, l_1 and l_2. Equations (4.35) also contain five different equations to determine M if k_1, k_2, l_1 and l_2 are known, for example, numerically as real and imaginary part of the roots of the $p(t)$ polynomial. Those of (4.35) corresponding to vanishing coefficients in the $p^{(4)}(t)$ polynomial do not give a solution for M. For monoclinic symmetry for instance, the right-hand sides of equations III and IV vanish when the tensor is referred to the symmetry coordinate system. Combining the two equations leads to the two restrictions for the roots: $(k_1^2 + l_1^2 - 1) = 0$ and $(k_2^2 + l_2^2 - 1) = 0$ or $k_1/l_1 = k_2/l_2$. This means that the norms of the roots are identically equal to one, or that the roots are along the same line in the complex plane. This is also in accordance with a later discussion of the multipoles for monoclinic symmetry.

We will now continue to find the expression A in (4.3). We have

$$\prod_{\nu=1}^{2}(a_\nu x + b_\nu y + c_\nu z) = (a_1 x + b_1 y + c_1 z)(a_2 x + b_2 y + c_2 z)$$

$$= (\hat{a}_1 x + \hat{b}_1 y + \hat{c}_1 z)(\hat{a}_2 x + \hat{b}_2 y + \hat{c}_2 z)[(a_1^2 + b_1^2 + c_1^2)(a_2^2 + b_2^2 + c_2^2)]^{1/2}$$

$$= A \prod_{\nu=1}^{2}(\hat{a}_\nu x + \hat{b}_\nu y + \hat{c}_\nu z),$$

where

$$A = [(a_1^2 + b_1^2 + c_1^2)(a_2^2 + b_2^2 + c_2^2)]^{1/2}$$

is the magnitude A in (4.3) for $q = 2$. Further we have, by using (4.18),

$$\begin{aligned} A &= M[(k_1^2 + l_1^2 + \tfrac{1}{4}(k_1^2 + l_1^2 - 1)^2)(k_2^2 + l_2^2 + \tfrac{1}{4}(k_2^2 + l_2^2 - 1)^2)]^{1/2} \\ &= \tfrac{1}{4}M(k_1^2 + l_1^2 + 1)(k_2^2 + l_2^2 + 1). \end{aligned} \tag{4.36}$$

Since M is expressed by the elastic constants in (4.35), it follows that A can be expressed by the elastic constants.

The harmonic tensor associated with the non-totally symmetric part of the hierarchically symmetric tensor is denoted by h_{ij}, and is given in Ch. 2 as

$$h_{ij} = \tfrac{2}{3}(\hat{C}_{ij} - \hat{V}_{ij}). \tag{4.37}$$

Substitution of (4.37) into (4.29) gives

$$\begin{aligned} a_4^{(h)} &= \tfrac{2}{3}[c_{44} - c_{55} + c_{13} - c_{23} - 2i(c_{36} - c_{45})], \\ a_3^{(h)} &= \tfrac{8}{3}[c_{25} - c_{46} - i(c_{14} - c_{56})], \\ a_2^{(h)} &= \tfrac{4}{3}[-c_{44} - c_{55} + 2c_{66} - 2c_{12} + c_{13} + c_{23}]. \end{aligned} \tag{4.38}$$

In calculating A we have similar equations to (4.35) to determine M. By using (4.34) and (4.38) we have

$$
\begin{aligned}
M(k_1k_2 - l_1l_2) &= \tfrac{2}{3}(c_{44} - c_{55} + c_{13} - c_{23}) \quad \mathrm{I} \\
M(k_1l_2 + l_1k_2) &= \tfrac{4}{3}(c_{36} - c_{45}) \quad \mathrm{II} \\
M((k_1^2 + l_1^2 - 1)k_2 + k_1(k_2^2 + l_2^2 - 1)] &= -\tfrac{16}{9}(c_{25} - c_{46}) \quad \mathrm{III} \\
M[(k_1^2 + l_1^2 - 1)l_2 + l_1(k_2^2 + l_2^2 - 1)] &= -\tfrac{16}{9}(c_{14} - c_{56}) \quad \mathrm{IV} \\
M[-2k_1k_2 - 2l_1l_2 + (k_1^2 + l_1^2 - 1)(k_2^2 + l_2^2 - 1)] &= \tfrac{4}{3}(-c_{44} - c_{55} \\
&\quad + 2c_{66} - 2c_{12} + c_{13} + c_{23}). \quad \mathrm{V} \qquad (4.39)
\end{aligned}
$$

Then (4.36) and (4.39) give the magnitude A expressed by the elastic constants.

4.4 Calculation of the magnitude A associated with H_{ijkl}

After the magnitude related to the two second degree harmonic polynomials are calculated, it is easy to find the magnitude associated to the fourth degree polynomial. However the calculation is tedious, and is given in the Appendix of this chapter. The magnitude is, according to (A.2), given as

$$A = \tfrac{1}{16}R(k_1^2 + l_1^2 + 1)(k_2^2 + l_2^2 + 1)(k_3^2 + l_3^2 + 1)(k_4^2 + l_4^2 + 1), \qquad (4.40)$$

where R is defined by the elastic constants (see the Appendix).

4.5 Classification of symmetry classes

In the following the polynomials $p^{(8)}(t)$, $p^{(H)}(t)$ and $p^{(h)}(t)$ are given for the different symmetry classes. The roots of a polynomial determine the corresponding multipole. For some symmetry classes, explicit expressions for the multipoles (relative to a symmetry coordinate system for the medium) are presented. The classification is summarized in Table 4.1.

Before giving the classification of the symmetry classes by means of the multipoles, some general comments on roots of our $p(t)$ polynomials are given.

If $z = k+il$ is a root, then also $-1/z^* = -(k+il)/(k^2+l^2)$ is a root. $|z|^2 = k^2+l^2$ and $|-1/z^*|^2 = 1/(k^2+l^2)$. The arguments of the two roots differ by π in the complex plane, and the norms of the roots are reciprocal. When one root is $z = k + il$, the components of the corresponding direction in the multipole is given in (4.18). Thus the horizontal projection of a direction in a multipole is proportional to the corresponding root z. Thus, to the roots z and $-1/z^*$, the arguments of the horizontal projections of the two related directions in the multipoles differ by π, and the lengths of the two directions are reciprocal of one another. Moreover, except for a positive scalar (see (4.18)), the z-component of the space direction determined by the root $-1/z^*$, is given by

$$c' = \tfrac{1}{2}[1 - (k^2 + l^2)]/(k^2 + l^2),$$

where c' has opposite sign of the z-component of the space direction determined by the root z. It is then easy to see that the direction determined by the roots z and $-1/z^*$ is represented by vectors symmetric about the origin. In the further discussion we define the two opposite vectors to determine one space direction in the multipole. The vertical component of a direction in a multipole is proportional to $\frac{1}{2}(k^2 + l^2 - 1)$. Thus if the norm of a root is equal to one, the vertical component of the related direction is equal to zero, so this specific direction in the bouquet is in the (x, y)-plane.

4.5.1 Monoclinic symmetry

The following elastic constants are identically zero when referred to the symmetry coordinate system with the z-axis as symmetry axis: c_{14}, c_{15}, c_{24}, c_{25}, c_{34}, c_{35}, c_{46} and c_{56}. The coefficients in $p^{(8)}(t)$ then become, from (4.27),

$$\begin{aligned}
a_8 &= c_{11} + c_{22} - 4c_{66} - 2c_{12} + 4i(-c_{16} + c_{26}),\\
a_6 &= 4[-c_{11} + c_{22} - 4c_{44} + 4c_{55} + 2c_{13} - 2c_{23} + 2i(c_{16} + c_{26} - 2c_{36} - 4c_{45})],\\
a_4 &= 2[3c_{11} + 3c_{22} + 8c_{33} - 16c_{44} - 16c_{55} + 4c_{66} + 2c_{12} - 8c_{13} - 8c_{23}],\\
a_7 &= a_5 = a_3 = a_1 = 0, \quad a_2 = a_6^*, \quad a_0 = a_8^*. \qquad (4.41)
\end{aligned}$$

Notice that the coefficients are generally complex. By a specific rotation of the coordinate system about the z-axis, the elastic constant c_{45} is equal to zero in the new coordinate system (**6**). This statement is true for c_{36} also. Thus monoclinic symmetry only has 12 independent constants.

From (4.41) the polynomial $p^{(8)}(t)$ becomes

$$p^{(8)}(t) = a_8 t^8 + a_6 t^6 + a_4 t^4 + a_6^* t^2 + a_8^* \qquad (4.42)$$

and corresponds to a fourth degree polynomial in $x = t^2$. This means that (4.42) has four pairs of roots in the complex plane. The arguments of the roots in each pair differ by π, and the roots have the same norm $|z|$. Since the roots in each pair have the same norm, they do not generally satisfy the condition: 'if z is a root of $p(t)$, then $-1/z^*$ is a root also'. This condition is satisfied only when the norms of the roots are identically one.

If the norm of one root is different from 1, there are in total four roots of $p^{(8)}(t)$ along the same line in the complex plane. These roots correspond to two directions in the multipole bouquet. These directions are symmetric about the z-axis. If in addition the norm of at least one more root is different from 1, the remaining four roots of $p^{(8)}(t)$ are along one line by similar arguments as above. The corresponding directions in the bouquet are along two lines, see Fig. 4.1a. In a possible degenerate case the two directions would be coincident.

If the norms of four roots are different from one, and the norms of the remaining four roots are equal to one, there are two directions in the symmetry plane, and two inclined directions in the multipole bouquet; see Fig. 4.1b. If the norm of the roots in all pairs of roots are equal to one, the eight roots are along four lines in the complex plane if there are no multiple roots. The four directions in the multipole are in the symmetry plane, see Fig. 4.1c.

In the case of more than two pairs of roots along the same line (degenerate case), all eight roots are along one line.

We have then shown that in all cases, except for degenerate cases, the directions in the multipole are along four lines. An interesting problem is to find out possible conditions on the elastic constants when we have degeneracy.

In all cases, for each direction in the multipole, there is one direction symmetric about the symmetry axis (the projections in the symmetry plane are along the same line).

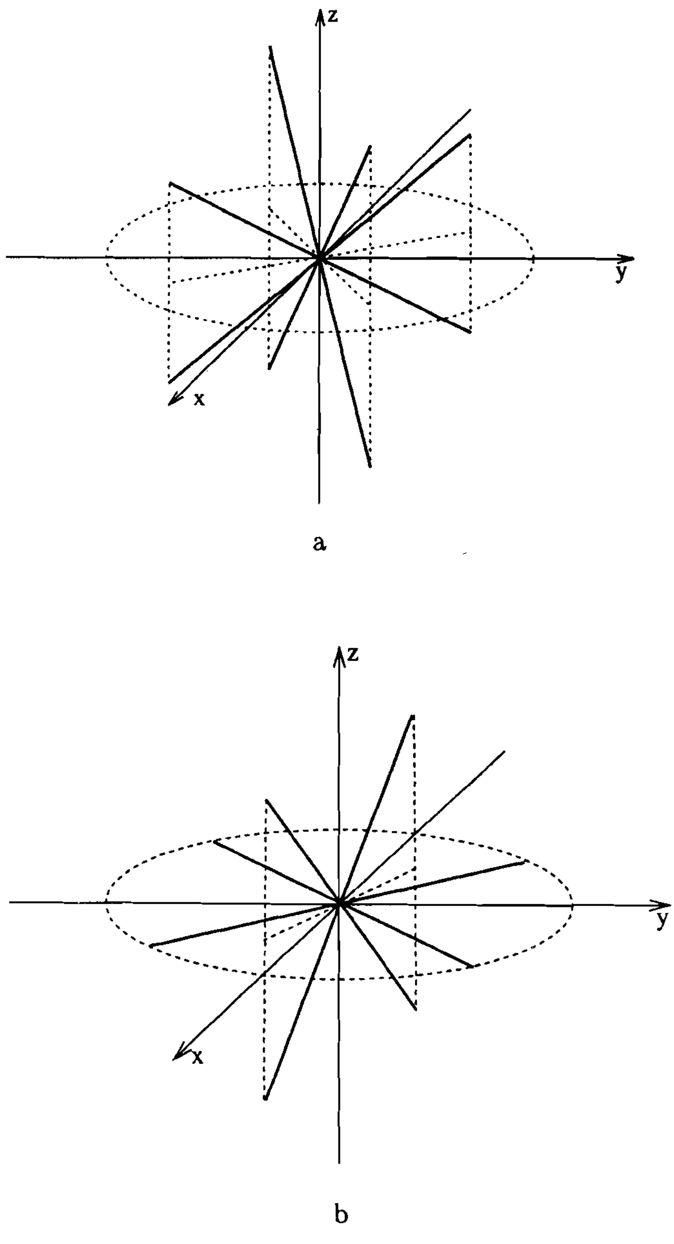
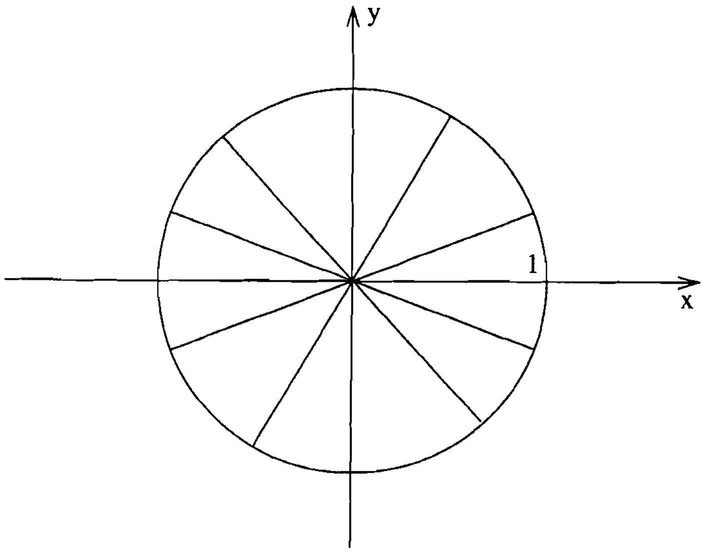


Fig. 4.1: Directions in the multipole for monoclinic symmetry. a) four inclined directions. b) two inclined directions and two perpendicular to the symmetry axis.



c

Fig. 4.1,c: Directions in the multipole for monoclinic symmetry. Four directions perpendicular to the symmetry axis.

For a specific chosen tensor of monoclinic symmetry (mono.q), see Fig. 4.2, where the z-axis is the symmetry axis, two of the directions in the multipole are perpendicular to the symmetry axis, see the later discussion of mono.q. The other two lines are inclined and symmetric about the symmetry axis.

$$\begin{pmatrix} 3.150 & 1.950 & 1.850 & 0.000 & 0.000 & 1.100 \\ & 2.750 & -1.350 & 0.000 & 0.000 & 1.000 \\ & & 6.650 & 0.000 & 0.000 & 2.000 \\ & & & 2.550 & 0.850 & 0.000 \\ & & & & 2.600 & 0.000 \\ & & & & & 2.450 \end{pmatrix}$$

Fig. 4.2: Tensor of monoclinic symmetry (mono.q). The z-axis is the symmetry axis.

For another tensor of monoclinic symmetry with symmetry axis in the z-direction, none of the directions is in the symmetry plane. However, in both cases the directions are symmetric about the z-axis.

We will now find the roots of the polynomial $p^{(H)}(t)$. None of the elastic coefficients in the expressions for $a_4^{(H)}$ and $a_2^{(H)}$ is identically equal to zero, thus $a_4^{(H)}$ and

$a_2^{(H)}$ are both generally different from zero, but $a_3^{(H)} = a_1^{(H)} = 0$. $a_4^{(H)}$ is complex. The polynomial $p^{(H)}(t)$ in (4.28) then becomes

$$p^{(H)}(t) = a_4^{(H)} t^4 + a_2^{(H)} t^2 + a_4^{(H)*}, \tag{4.43}$$

where $a_4^{(H)}$ and $a_2^{(H)}$ are given in (4.31). The equation $p^{(H)}(t) = 0$ corresponds to a second order equation in $w = t^2$. The two roots in

$$a_4^{(H)} w^2 + a_2^{(H)} w + a_4^{(H)*} = 0 \tag{4.44}$$

correspond to two pairs of roots of (4.43). The arguments of the roots in each pair differ by π, and the roots have the same norm. The roots connected by the condition 'if z is a root of $p(t)$, then $-1/z^*$ is a root also' are along the same line in the complex plane as well. Generally (except when the norm is equal to 1), all four roots have to be along one line in the complex plane according to the arguments applied to the roots of $p^{(8)}(t)$. The horizontal projections in the symmetry plane of the two directions in the multipole differ by π, and the angles to the z-axis are the same for the two directions.

In the special case where the norms of the roots are equal to one, the roots are generally along two lines in the complex plane. In this case the multipole consists of two directions in the (x, y)-plane. In the following it is shown under which conditions the norm of the roots of (4.43) are equal to one. For simplicity, write (4.44) as $aw^2 + bw + a^* = 0$, where $a = a_4^{(H)}$, and $b = a_2^{(H)}$ is a real constant. The solution is given as

$$w = \tfrac{1}{2}(-b \pm \delta^{1/2}) a^*/|a|^2 \quad \text{with} \quad \delta = b^2 - 4|a|^2.$$

There are three possibilities for the solution, depending on the sign of δ.

1. $\delta < 0$:
$$w = \tfrac{1}{2}[-b \pm i(-\delta)^{1/2}] a^*/|a|^2.$$
Thus, $|w| = |t^2| = |t||t| = 1$, and so in this case the norm of the root of (4.43) is equal to one.

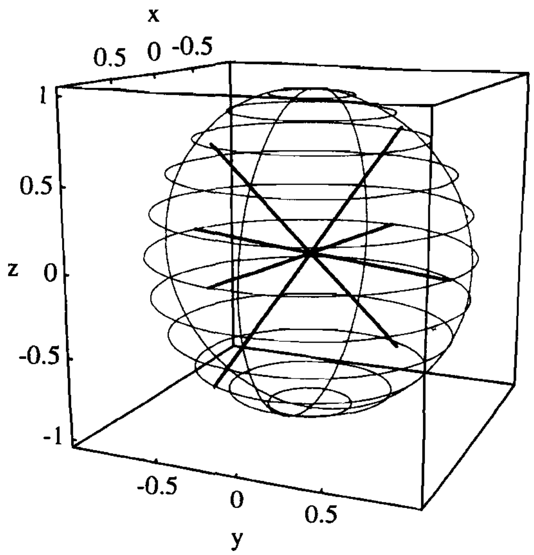
2. $\delta > 0$:
$$w = \tfrac{1}{2}(-b \pm \delta^{1/2}) a^*/|a|^2.$$
This is generally complex. Also, $|w| = \frac{1}{2}| - b \pm \delta^{1/2}|/|a| \neq 1$.

3. $\delta = 0$:
$$w = -\tfrac{1}{2} b/a \quad \text{and} \quad |w| = \tfrac{1}{2}|b|/|a| \neq 1.$$

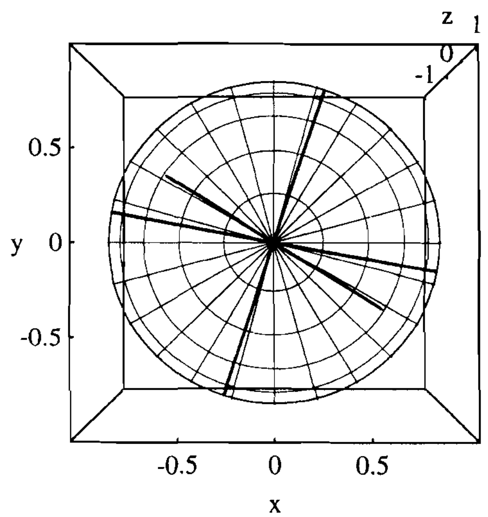
For the polynomial $p^{(h)}(t)$, we have the similar situation as for $p^{(H)}(t)$. The arguments and conclusion are the same as above, but the roots of the two polynomials are of course generally different.

Example 2

Let us study the multipoles for the fourth rank tensor H_{ijkl} of monoclinic symmetry with z-axis as symmetry axis (mono.q), see Fig. 4.2. Let H_{ijkl} be denoted by $H^{(4)}$, and further let the second rank tensors H_{ij} and h_{ij} be denoted by $H^{(2)}$ and $h^{(2)}$, respectively. The display of directions in the multipoles is done by using MATHEMATICA. Fig. 4.3 shows the bouquet of directions in the multipole of $H^{(4)}$ together with a transparent sphere.

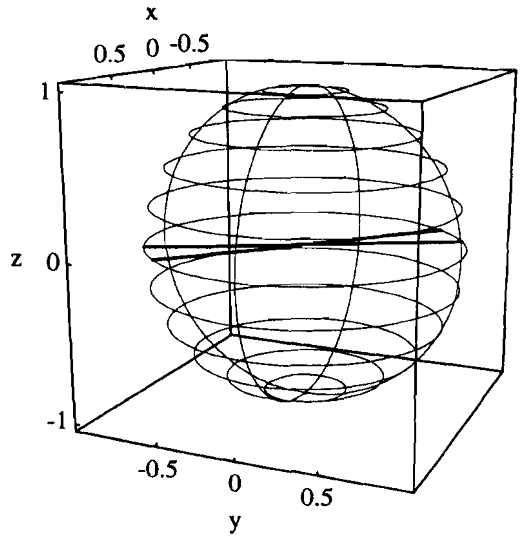


a

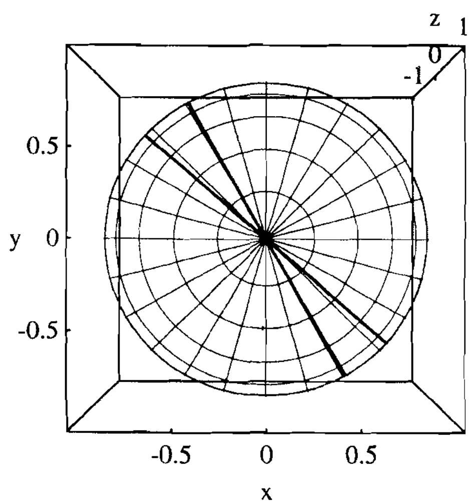


b

Fig. 4.3: H-4 multipoles, monoclinic symmetry. In b the viewpoint is on the symmetry axis.

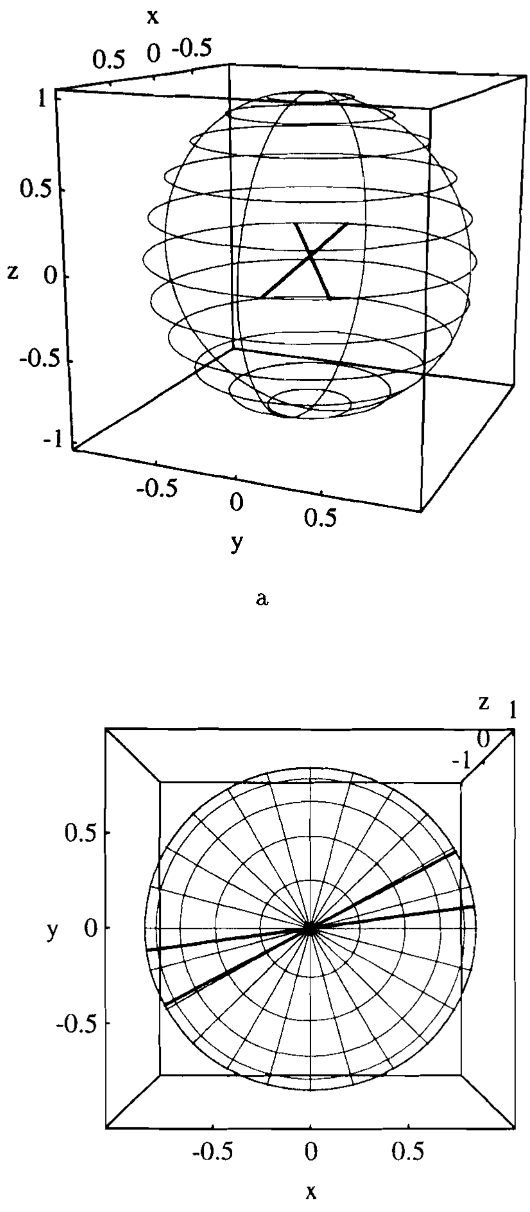


a



b

Fig. 4.4: H-2 multipoles, monoclinic symmetry. In b the viewpoint is on the symmetry axis.



a

b

Fig. 4.5: h-2 multipoles, monoclinic symmetry. In b the viewpoint is on the symmetry axis.

There are four directions, in this case two directions in the symmetry plane, and two inclined relative to the symmetry axis. For each of the directions, there is one symmetric about the z-axis. In Fig. 4.3b the viewpoint is a point on the z-axis. The two directions which are not in the symmetry plane have identical projections in the symmetry plane. By calculation, this projection deviates $-32.3°$ (or $-32.3° + 180°$) from the x-axis. Positive angle is defined counterclockwise. The two horizontal directions deviate $-10.6°$ and $72.1°$ respectively.

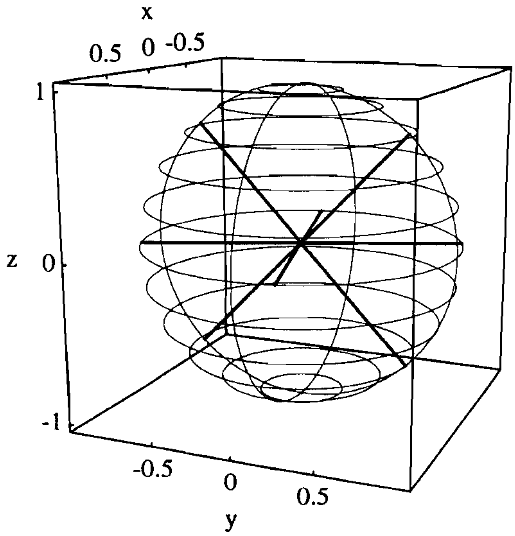
Fig. 4.4 shows the $H^{(2)}$ multipole. In Fig. 4.4b the viewpoint is at the z-axis. Both directions are in the symmetry plane. The deviation from the x-axis for the two directions is $-41.5°$ and $-61.2°$ respectively. The average value is $-51.3°$, and one perpendicular makes $38.7°$ with the x-axis.

Similar to Fig. 4.4, Fig. 4.5 shows the $h^{(2)}$ multipole which is in the symmetry plane as well. The deviations from the x-axis for the two directions are $7.8°$ and $28.4°$. The average value of the two is $18.1°$, which coincides with an eigenvector of the second rank tensor associated to the non- totally symmetric part of the hierarchically symmetric tensor (A_{ijkl}, see Ch. 2). A theoretical discussion of connections between multipole directions and eigenvectors of different second rank tensors associated with the hierarchically symmetric tensor is left for further development.

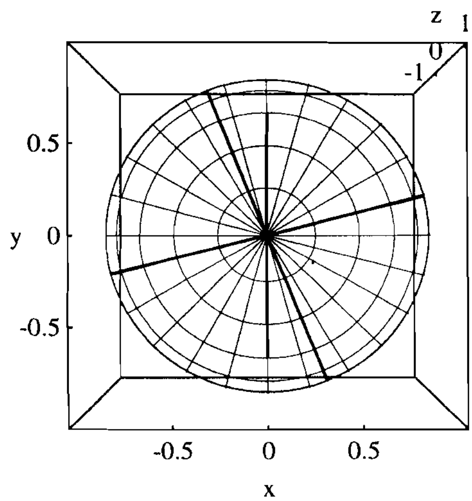
There is one common symmetry axis for directions in the multipoles, which is the z-axis (the monoclinic symmetry axis).

If the tensor is referred to a coordinate system rotated by $44.16°$ about the z-axis, the elastic constant c_{45} is equal to zero in the new coordinate system (**6**). By a similar rotation of $25.67°$, the elastic constant c_{36} is equal to zero in the new coordinate system. The bouquet of directions in the multipole is rotated the same amount as well, and no directions in the multipoles (or their average directions) are parallel to the new coordinate axes.

Fig. 4.6 shows the $H^{(4)}$ multipole for the monoclinic tensor referred to a coordinate system rotated by $-122.3°$ about the z-axis. The inclined directions in the multipole are then in the new (y, z)-plane. The bouquet of directions in Fig. 4.3 is rotated by an amount of $122.3°$ as expected. When the tensor is referred to a coordinate system which in addition is rotated by $15°$ about the new x-axis, the tensor has 21 elastic constants. Viewed from a point on an axis tilted relative to the symmetry axis, we get a picture like Fig. 4.7 for the directions in the $H^{(4)}$ multipole. The figure shows that the two inclined up-pointing directions are inclined about $28°$ in the negative y-direction and about $60°$ in the positive y-direction respectively. The average value is $16°$ in the positive y-direction. Expected values should be $28°$ and $58°$, respectively, which are the calculated values (average value: $15°$). The figure illustrates that in this case it was possible to find the direction of the symmetry axis by using a suitable viewpoint. A further development is left for a more detailed description of how to find the orientation of symmetry elements.



a



b

Fig. 4.6: H-4 multipoles for mono.q in a coordinate system rotated -122.3 degrees about the symmetry axis. In b the viewpoint is on the symmetry axis.

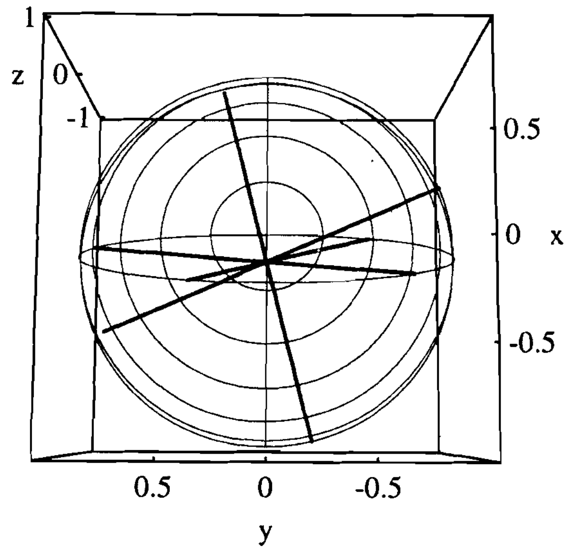


Fig. 4.7: H-4 multipoles for mono.q in a coordinate system rotated -122.3 degrees about the z-axis and 15 degrees about the new x-axis. The tensor has 21 elastic components. In b the viewpoint is on the symmetry axis.

4.5.2 Trigonal symmetry

The following elastic constants are identically equal to zero when referred to the symmetry coordinate system with the 3-axis as symmetry axis: c_{16}, c_{26}, c_{34}, c_{35}, c_{36} and c_{45}. In addition there are the following relations:

$$c_{22} = c_{11}, \quad c_{23} = c_{13}, \quad c_{24} = -c_{14}, \quad c_{25} = -c_{15},$$

$$c_{55} = c_{44}, \quad c_{66} = \tfrac{1}{2}(c_{11} - c_{12}), \quad c_{46} = -c_{15}, \quad c_{56} = c_{14}.$$

The non-zero coefficients in the eighth order polynomial are

$$a_7 = 4(8c_{15} - ic_{14}), \quad a_4 = 16(c_{11} + c_{33} - 4c_{44} - 2c_{13}), \quad a_1 = -a_7^*.$$

The polynomial then becomes

$$p^{(8)}(t) = a_7t^7 + a_4t^4 - a_7^*t = t(a_7t^6 + a_4t^3 - a_7^*). \tag{4.45}$$

Thus $t = 0$ is one root of the polynomial $p^{(8)}(t)$. This root corresponds to the z-axis, that is the symmetry axis, as one of the directions in the bouquet. The other roots of $p^{(8)}(t)$ are obtained by substiting $t^3 = w$ and solving

$$a_7w^2 + a_4w - a_7^* = 0. \tag{4.46}$$

To each of the two roots in (4.46) corresponds three complex solutions of $p^{(8)}(t) = 0$. All three roots of (4.45) corresponding to each solution of (4.46) have the same norm, and differ in argument by $2\pi/3$ in the complex plane. Each of the two sets of the three solutions are related by the condition: 'if z is a root of $p(t,1)$, then $-1/z^*$ is a root also', in the way that the roots are along three lines in the complex plane. The multipole than consists of one direction along the symmetry axis, and three directions whose horizontal components differ by $2\pi/3$. The angles to the z-axis is equal for the three directions, and depend on the elastic constants.

In the polynomials $p^{(H)}(t)$ and $p^{(h)}(t)$ the coefficients $a_4^{(H)}$, $a_3^{(H)}$, $a_4^{(h)}$ and $a_3^{(h)}$ are equal to zero. We than have

$$p^{(H)}(t) = a_2^{(H)}t^2 \quad \text{with} \quad a_2^{(H)} = \tfrac{4}{21}[-4c_{11} + 3c_{33} + 2c_{44} + c_{13}] \tag{4.47}$$

and

$$p^{(h)}(t) = a_2^{(h)}t^2 \quad \text{with} \quad a_2^{(h)} = \tfrac{4}{3}[c_{11} - 2c_{44} - 3c_{12} + 2c_{13}]; \tag{4.48}$$

$z = 0$ is a double root in the polynomials. Thus the two directions in the multipole corresponding to each of the two polynomials (4.47) and (4.48) are parallel to the symmetry axis (z-axis).

4.5.3 Tetragonal symmetry

The following elastic constants are identically equal to zero: c_{14}, c_{15}, c_{24}, c_{25}, c_{34}, c_{35}, c_{36}, c_{45}, c_{46} and c_{56}. In addition there are the following relations between the remaining elastic constants:

$$c_{22} = c_{11}, \quad c_{23} = c_{13}, \quad c_{26} = -c_{16} \quad \text{and} \quad c_{55} = c_{44}.$$

The non-vanishing coefficients in the eighth degree polynomial are

$$a_8 = 2c_{11} - 4c_{66} - 2c_{12} - 8ic_{16}, \quad a_0 = a_8^*,$$

$$a_4 = 12c_{11} + 16c_{33} - 64c_{44} + 8c_{66} + 4c_{12} - 32c_{13}.$$

The polynomial then becomes

$$p^{(8)}(t) = a_8t^8 + a_4t^4 + a_8^*. \tag{4.49}$$

By substituting $t^4 = w$, and solving the second order equation

$$a_8w^2 + a_4w + a_8^* = 0 \tag{4.50}$$

we generally get two solutions of (4.50). Each of the two solutions corresponds to four roots of the eighth degree polynomial (4.49). Each of the corresponding sets of four roots of (4.49) has the same norm, and are separated by $\pi/2$ in the complex plane. Thus the projections in the horizontal plane of the directions in the bouquet are separated by $\pi/2$. The angles to the z-axis are equal for the four directions, and depends on the elastic constants. A discussion using arguments similar to previous arguments leads to the fact that the four directions above are the only directions in the bouquet.

The polynomials $p^{(H)}(t)$ and $p^{(h)}(t)$ are of second order as for trigonal symmetry. The coefficients are given by

$$a_2^{(H)} = \tfrac{4}{21}[-3c_{11} + 3c_{33} + 2c_{44} - 2c_{66} - c_{12} + c_{13}]$$

and

$$a_2^{(h)} = \tfrac{8}{3}[-c_{44} + c_{66} - c_{12} - c_{13}].$$

The two directions in the multipole are parallel to the symmetry axis (z-axis) (the roots are zero) for the multipoles corresponding to both polynomials.

4.5.4 Hexagonal symmetry

The following elastic constants are identically equal to zero: c_{14}, c_{15}, c_{16}, c_{24}, c_{25}, c_{26}, c_{34}, c_{35}, c_{36}, c_{45}, c_{46} and c_{56}. There are the following relations between elastic constants:

$$c_{22} = c_{11}, \quad c_{23} = c_{13}, \quad c_{55} = c_{44}, \quad c_{66} = \tfrac{1}{2}(c_{11} - c_{12}).$$

The only non-zero coefficient in the eighth order polynomial is

$$a_4 = 16(c_{11} + c_{33} - 4c_{44} - 2c_{13}).$$

The polynomial then becomes $p^{(8)}(t) = a_4 t^4$. The only root is $t = 0$ which corresponds to directions in the bouquet parallel to the symmetry axis.

For hexagonal symmetry, as for trigonal and tetragonal symmetry, the polynomials $p^{(H)}(t)$ and $p^{(h)}(t)$ are of second degree. The coefficients are

$$a_2^{(H)} = \tfrac{2}{21}[-5c_{11} - 3c_{22} + 6c_{33} + 4c_{44} + 2c_{13}],$$

$$a_2^{(h)} = \tfrac{4}{3}[c_{11} - 2c_{44} - 3c_{12} + 2c_{13}].$$

The two directions in the multipole are parallel to the symmetry axis (z-axis) for the multipole corresponding to each polynomial.

4.5.5 Orthorhombic symmetry

For orthorhombic symmetry, at most nine independent elastic components are different from zero. They are: $c_{11}, c_{22}, c_{33}, c_{44}, c_{55}, c_{66}, c_{12}, c_{13}$ and c_{23}. The non-vanishing coefficients in the eighth degree polynomial are

$$a_8 = a_0 = c_{11} + c_{22} - 4c_{66} - 2c_{12},$$

$$a_6 = a_2 = 4(-c_{11} + c_{22} - 4c_{44} + 4c_{55} + 2c_{13} - 2c_{23}),$$

$$a_4 = 2(3c_{11} + 3c_{22} + 8c_{33} - 16c_{44} - 16c_{55} + 4c_{66} + 2c_{12} - 8c_{13} - 8c_{23}).$$

The polynomial then becomes

$$p^{(8)}(t) = a_8 t^8 + a_6 t^6 + a_4 t^4 + a_6 t^2 + a_8. \tag{4.51}$$

As for monoclinic symmetry, the polynomial corresponds to a fourth degree polynomial in $w = t^2$. This means that there are four pairs of roots in (4.51) in the complex plane. Unlike the monoclinic symmetry, the coefficients are real. Thus the roots of the fourth degree polynomial in w consist of two complex conjugated pairs. This means that the roots in w occur symmetrically about the x-axis in the complex plane. To each w corresponds two roots of the eighth degree polynomial differing by π ($w = t^2$). Thus the eight roots occur symmetrically about the two axes in the complex plane. Following similar arguments as for monoclinic symmetry, the projection of the directions in the bouquet also occur symmetrically about the x- and y-axes, and there are at most four directions in the bouquet. Conjugate pairs implies that rotation about the x-axis by π brings a direction in the bouquet into the direction determined by the conjugate root. Symmetry about the y-axis guarantees invariance of the bouquet against rotation of π about the y-axis. To find further properties of the multipole, solution of the fourth order equation is necessary.

For the polynomials $p^{(H)}(t)$ and $p^{(h)}(t)$, $a_3^{(H)}$ and $a_3^{(H)}$ are equal to zero. The rest of the polynomials are given by

$$a_4^{(H)} = \tfrac{1}{21}[3c_{11} - 3c_{22} - 2c_{44} + 2c_{55} + c_{13} - c_{23}],$$

$$a_2^{(H)} = \tfrac{2}{21}[-3c_{11} - 3c_{22} + 6c_{33} + 2c_{44} + 2c_{55} - 4c_{66} - 2c_{12} + c_{13} + c_{23}],$$

$$a_4^{(h)} = \tfrac{2}{3}[c_{44} - c_{55} + c_{13} - c_{23}],$$

$$a_2^{(h)} = \tfrac{4}{3}[-c_{44} - c_{55} + 2c_{66} - 2c_{12} + c_{13} + c_{23}].$$

The second degree polynomials (4.28) then become

$$p^{(H)}(t) = a_4^{(H)} t^4 + a_2^{(H)} t^2 + a_4^{(H)*} \quad \text{and} \quad p^{(h)}(t) = a_4^{(h)} t^4 + a_2^{(h)} t^2 + a_4^{(h)*}.$$

For both polynomials, the coefficients are real, thus complex roots of each of the second order polynomials in $w = t^2$ occur conjugated. Each of the two roots corresponds to two roots in t with arguments differing by π. If the norms of the four roots are equal to one, the multipole generally consists of two horizontal directions. If the norms are different from one, the roots are along one line in the complex plane, and the horizontal projection of the directions are along the same line. Regardless of the norm, the multipoles consist of two directions. Only explicit expressions for the roots will give more details.

4.5.6 Cubic symmetry

For cubic symmetry, there are three independent elastic constants, and we have the following relations between the non-vanishing constants:

$$c_{22} = c_{33} = c_{11}, \quad c_{13} = c_{23} = c_{12} \quad \text{and} \quad c_{44} = c_{55} = c_{66}.$$

The non-vanishing coefficients in the eighth degree polynomial are

$$a_8 = 2(c_{11} - 2c_{66} - c_{12}), \quad a_4 = 14a_8 \quad \text{and} \quad a_0 = a_8.$$

The polynomial

$$p^{(8)}(t) = a_8 t^8 + 14a_8 t^4 + a_8 \tag{4.52}$$

corresponds to a second degree polynomial in $w = t^4$. Since a_8 is a common factor of the polynomial, the roots are independent of the elastic constants. The roots of the second order polynomial in w are

$$w_1 = -7 + 4 \cdot 3^{1/2} \quad \text{and} \quad w_2 = -7 - 4 \cdot 3^{1/2}.$$

To each of the two values of w corresponds four values of t since $w = t^4$. If $\phi = \pi/4$, the eight roots of (4.52) corresponding to w_1 and w_2 have arguments ϕ, 3ϕ, 5ϕ and 7ϕ in the complex plane. These are also the arguments of the horizontal projections of the corresponding directions in the multipole. The four roots of the polynomial (4.52) corresponding to $w_1 = -7 + 4 \cdot 3^{1/2}$ are:

$$z_1 = (7 - 4 \cdot 3^{1/2})^{1/4} e^{i\phi} = 0.366 + i0.366,$$

$$z_2 = (7 - 4 \cdot 3^{1/2})^{1/4} e^{i3\phi} = -0.366 + i0.366,$$

$$z_3 = (7 - 4 \cdot 3^{1/2})^{1/4} e^{i5\phi} = -0.366 - i0.366,$$

$$z_4 = (7 - 4 \cdot 3^{1/2})^{1/4} e^{i7\phi} = 0.366 - i0.366.$$

The corresponding directions in the multipole are thus given by (4.18):

$$(-0.366, -0.366, -0.366), \quad (0.366, -0.366, -0.366),$$

$$(0.366, 0.366, -0.366), \quad (-0.366, 0.366, -0.366).$$

Thus the four directions are along the diagonals in a cube, and make an angle of 54.7° against the z-axis.

The four roots corresponding to $w_2 = -7 - 4 \cdot 3^{1/2}$ are:

$$z_5 = (7 + 4 \cdot 3^{1/2})^{1/4} e^{i\phi} = 1.366 + i1.366,$$

$$z_6 = (7 + 4 \cdot 3^{1/2})^{1/4} e^{i3\phi} = -1.366 + i1.366,$$

$$z_7 = (7 + 4 \cdot 3^{1/2})^{1/4} e^{i5\phi} = -1.366 - i1.366,$$

$$z_8 = (7 + 4 \cdot 3^{1/2})^{1/4} e^{i7\phi} = 1.366 - i1.366.$$

The corresponding directions in the multipole are thus given by (4.18):

$$(-1.366, -1.366, 1.366), \quad (1.366, -1.366, 1.366),$$

$$(1.366, 1.366, 1.366), \quad (-1.366, 1.366, 1.366).$$

Thus the four directions are along the diagonals in a cube, as above.

As one of the referees pointed out, from the numerical values of z_i, for example z_1 and z_5, we see the relation

$$(7/4 + 3^{1/2})^{1/4} - (7/4 - 3^{1/2})^{1/4} = 1, \tag{4.53}$$

which can easily be verified.

The eight z_i have to satisfy the condition *if* z *is a root of* $p^{(2q)}(t)$, *then* $-1/z^*$ *is a root also.* z_1 and z_5 are related by $z_5 = 1/z_1^*$, and (4.53) expresses the following properties of the roots of $p^{(8)}(t)$:

$$\mathrm{Re}(z) - \mathrm{Re}(1/z^*) = \pm 1 \quad \text{and} \quad \mathrm{Im}(z) - \mathrm{Im}(1/z^*) = \pm 1.$$

For the polynomials $p^{(H)}$ and $p^{(h)}$, all the coefficients are equal to zero, so there are no multipoles corresponding to the harmonic tensors $H^{(2)}$ and $h^{(2)}$.

4.5.7 Isotropic symmetry

For isotropic symmetry, there are two independent elastic constants, and we have the following relations between the non-vanishing constants:

$$c_{22} = c_{33} = c_{11}, \quad c_{13} = c_{23} = c_{12} \quad \text{and} \quad c_{44} = c_{55} = c_{66} = \tfrac{1}{2}(c_{11} - c_{12}).$$

The coefficients in the three polynomials: eighth order polynomial, $p^{(H)}$ and $p^{(h)}$, are zero. This means that there are no multipoles corresponding to the harmonic tensors $H^{(4)}$, $H^{(2)}$ and $h^{(2)}$.

4.6 Conclusion

A classification of symmetry classes of the hierarchically symmetric tensor is presented by means of bouquets of space directions. The analysis is based on harmonic decomposition of the hierarchically symmetric tensor presented by Backus (**1**) and further developed in Ch. 2. Explicit expressions for the bouquets of space directions related to the harmonic tensors are given. Software is developed to calculate the bouquets of space directions, and MATHEMATICA is used for displaying.

As a demonstration of the method, multipoles for a specific tensor of monoclinic symmetry are displayed, also when the coordinates are not the symmetry coordinate system. The space directions are related to the symmetry of the tensor, and are independent of coordinate system. The directions occur as pairs symmetric about

Symmetry	$H^{(4)}$	$H^{(2)}$	$h^{(2)}$
Monoclinic	4 directions. Symmetric about symmetry axis. Pairs of inclined directions define planes containing symmetry axis.	2 directions. Symmetric about symmetry axis.	2 directions. Symmetric about symmetry axis.
Orthorhombic	4 directions. 3 symmetry axes.	2 directions. Symmetry about the same axes as for $H^{(4)}$.	2 directions. Symmetry about the same axes as for $H^{(4)}$.
Tetragonal	4 directions. 2 pairs of directions defining 2 planes differing 90°.	1 direction, parallel to symmetry axis.	1 direction, parallel to symmetry axis.
Cubic	4 directions. Parallel to the diagonals in a cube.	None	None
Trigonal	4 directions. 1 parallel to symmetry axis. 3 whose horizontal projections differ 120°.	1 direction, parallel to symmetry axis.	1 direction, parallel to symmetry axis.
Hexagonal	1 direction, parallel to symmetry axis.	1 direction, parallel to symmetry axis.	1 direction, parallel to symmetry axis.
Isotropic	None	None	None

Table 4.1: Multipoles for different symmetry classes.

the symmetry axis defined by the tensor. This property can be used to determine the symmetry axis of an elastic medium.

Several questions are left for further development. Under which conditions on the elastic constants are there special arrangements of the multipoles for for example monoclinic symmetry? How does the method work for experimental elastic tensors?

Acknowledgements

I would like to thank Professor emeritus Dr. K. Helbig for all his support, encouragement and discussions. He is also thanked for the opportunity to use software developed by him. In addition the following persons at mathematical institutes are thanked for fruitful discussions: Dr. W.L.J. van den Kallen at the University of Utrecht, Professor Dr. H. Tverberg at the University of Bergen, Dr. K. Ranestad at the University of Oslo, and my colleague Dr. M. Dale. I would also like to thank two referees for their comments, and specially one of them who pointed out a couple of relations.

APPENDIX. Calculation of the magnitude A associated with H_{ijkl}.

From (4.14) and (4.32) we have

$$p^{(8)} = \prod_{\nu=1}^{4}(r_\nu\xi + s_\nu\eta)(s_\nu^*\xi - r_\nu^*\eta)$$

$$\begin{aligned}
&= [-k_1r_1r_1^*(\xi^2-\eta^2) + l_1r_1r_1^*i(\xi^2+\eta^2) + \tfrac{1}{2}(k_1^2+l_1^2-1)r_1r_1^*(2\xi\eta)] \\
&\times[-k_2r_2r_2^*(\xi^2-\eta^2) + l_2r_2r_2^*i(\xi^2+\eta^2) + \tfrac{1}{2}(k_2^2+l_2^2-1)r_2r_2^*(2\xi\eta)] \\
&\times[-k_3r_3r_3^*(\xi^2-\eta^2) + l_3r_3r_3^*i(\xi^2+\eta^2) + \tfrac{1}{2}(k_3^2+l_3^2-1)r_3r_3^*(2\xi\eta)] \\
&\times[-k_4r_4r_4^*(\xi^2-\eta^2) + l_4r_4r_4^*i(\xi^2+\eta^2) + \tfrac{1}{2}(k_4^2+l_4^2-1)r_4r_4^*(2\xi\eta)]
\end{aligned} \tag{A.1}$$

Using (4.33), we see that the first two of the four factors in (A.1) can be written as

$$\begin{gathered}
M[k_1k_2 - l_1l_2 - i(k_1l_2 + l_1k_2)]t^4 \\
+M[-(k_1^2+l_1^2-1)k_2 - k_1(k_2^2+l_2^2-1) + i((k_1^2+l_1^2-1)l_2 + l_1(k_2^2+l_2^2-1))]t^3 \\
+M[-2k_1k_2 - 2l_1l_2 + (k_1^2+l_1^2-1)(k_2^2+l_2^2-1)]t^2 \\
+M[(k_1^2+l_1^2-1)k_2 + k_1(k_2^2+l_2^2-1) + i((k_1^2+l_1^2-1)l_2 + l_1(k_2^2+l_2^2-1))]t \\
+M[k_1k_2 - l_1l_2 + i(k_1l_2 + l_1k_2)].
\end{gathered}$$

After multiplying two expressions similar to the one above, we obtain the eighth degree polynomial $p^{(8)}(t)$:

$$p^{(8)}(t) = \{M[k_1k_2 - l_1l_2 - i(k_1l_2 + l_1k_2)]t^4$$
$$+M[-(k_1^2 + l_1^2 - 1)k_2 - k_1(k_2^2 + l_2^2 - 1) + i((k_1^2 + l_1^2 - 1)l_2 + l_1(k_2^2 + l_2^2 - 1))]t^3$$
$$+M[-2k_1k_2 - 2l_1l_2 + (k_1^2 + l_1^2 - 1)(k_2^2 + l_2^2 - 1)]t^2$$
$$+M[(k_1^2 + l_1^2 - 1)k_2 + k_1(k_2^2 + l_2^2 - 1) + i((k_1^2 + l_1^2 - 1)l_2 + l_1(k_2^2 + l_2^2 - 1))]t$$
$$+M[k_1k_2 - l_1l_2 + i(k_1l_2 + l_1k_2)]\}\{N[k_3k_4 - l_3l_4 - i(k_3l_4 + l_3k_4)]t^4$$
$$+N[-(k_3^2 + l_3^2 - 1)k_4 - k_3(k_4^2 + l_4^2 - 1) + i((k_3^2 + l_3^2 - 1)l_4 + l_3(k_4^2 + l_4^2 - 1))]t^3$$
$$+N[-2k_3k_4 - 2l_3l_4 + (k_3^2 + l_3^2 - 1)(k_4^2 + l_4^2 - 1)]t^2$$
$$+N[(k_3^2 + l_3^2 - 1)k_4 + k_3(k_4^2 + l_4^2 - 1) + i((k_3^2 + l_3^2 - 1)l_4 + l_3(k_4^2 + l_4^2 - 1))]t$$
$$+N[k_3k_4 - l_3l_4 + i(k_3l_4 + l_3k_4)]\}$$

where $N = r_3r_3^*r_4r_4^*$. This polynomial shows the same relation between coefficients as we obtained in the development of $p^{(8)}(t)$ in (4.26), namely

$$a_3 = -a_5^*, \quad a_2 = a_6^*, \quad a_1 = -a_7^* \quad \text{and} \quad a_0 = a_8^*.$$

Rearrangement and ordering gives the coefficients of the polynomial. Explicit expressions for two of the coefficients are given below, where we use the notation $MN = R$:

$$\begin{aligned}
a_8 &= R\{k_1k_2k_3k_4 + l_1l_2l_3l_4 - k_1k_2l_3l_4 - l_1l_2k_3k_4 - k_1l_2k_3l_4 \\
&\quad - l_1k_2l_3k_4 - k_1l_2l_3k_4 - l_1k_2k_3l_4 - i[k_1k_2k_3l_4 + k_1k_2l_3k_4 \\
&\quad - l_1l_2l_3k_4 - l_1l_2k_3l_4 + k_1l_2k_3k_4 + l_1k_2k_3k_4 - k_1l_2l_3l_4 - l_1k_2l_3l_4]\} \\
a_7 &= R\{(k_1^2 + l_1^2 - 1)(-k_2k_3k_4 + k_2l_3l_4 + l_2k_3l_4 + l_2l_3k_4) \\
&\quad + (k_2^2 + l_2^2 - 1)(-k_1k_3k_4 + k_1l_3l_4 + l_1k_3l_4 + l_1l_3k_4) \\
&\quad + (k_3^2 + l_3^2 - 1)(-k_1k_2k_4 + k_1l_2l_4 + l_1k_2l_4 + l_1l_2k_4) \\
&\quad + (k_4^2 + l_4^2 - 1)(-k_1k_2k_3 + k_1l_2l_3 + l_1k_2l_3 + l_1l_2k_3) \\
&\quad + i[(k_1^2 + l_1^2 - 1)(-l_2l_3l_4 + l_2k_3k_4 + k_2l_3k_4 + k_2k_3l_4) \\
&\quad + (k_2^2 + l_2^2 - 1)(-l_1l_3l_4 + l_1k_3k_4 + k_1l_3k_4 + k_1k_3l_4) \\
&\quad + (k_3^2 + l_3^2 - 1)(-l_1l_2l_4 + l_1k_2k_4 + k_1l_2k_4 + k_1k_2l_4) \\
&\quad + (k_4^2 + l_4^2 - 1)(-l_1l_2l_3 + l_1k_2k_3 + k_1l_2k_3 + k_1k_2l_3)]\}
\end{aligned}$$

Comparing the coefficients above with the coefficients of $p^{(8)}(t)$ in (4.27), gives

$$\begin{aligned}
&R[k_1k_2k_3k_4 + l_1l_2l_3l_4 - k_1k_2l_3l_4 - l_1l_2k_3k_4 - k_1l_2k_3l_4 \\
&- l_1k_2l_3k_4 - k_1l_2l_3k_4 - l_1k_2k_3l_4] = c_{11} + c_{22} - 4c_{66} - 2c_{12} \qquad \text{I} \\
&R[k_1k_2k_3l_4 + k_1k_2l_3k_4 - l_1l_2l_3k_4 - l_1l_2k_3l_4 + k_1l_2k_3k_4 \\
&+ l_1k_2k_3k_4 - k_1l_2l_3l_4 - l_1k_2l_3l_4] = 4(c_{16} - c_{26}) \qquad \text{II} \\
&R[(k_1^2 + l_1^2 - 1)(-k_2k_3k_4 + k_2l_3l_4 + l_2k_3l_4 + l_2l_3k_4) \\
&+ (k_2^2 + l_2^2 - 1)(-k_1k_3k_4 + k_1l_3l_4 + l_1k_3l_4 + l_1l_3k_4) \\
&+ (k_3^2 + l_3^2 - 1)(-k_1k_2k_4 + k_1l_2l_4 + l_1k_2l_4 + l_1l_2k_4) \\
&+ (k_4^2 + l_4^2 - 1)(-k_1k_2k_3 + k_1l_2l_3 + l_1k_2l_3 + l_1l_2k_3)] = 8(c_{15} - c_{25} - 2c_{46}) \qquad \text{III}
\end{aligned}$$

$$\begin{aligned}
&R[(k_1^2+l_1^2-1)(-l_2l_3l_4+l_2k_3k_4+k_2l_3k_4+k_2k_3l_4)\\
&+(k_2^2+l_2^2-1)(-l_1l_3l_4+l_1k_3k_4+k_1l_3k_4+k_1k_3l_4)\\
&+(k_3^2+l_3^2-1)(-l_1l_2l_4+l_1k_2k_4+k_1l_2k_4+k_1k_2l_4)\\
&+(k_4^2+l_4^2-1)(-l_1l_2l_3+l_1k_2k_3+k_1l_2k_3+k_1k_2l_3)]\\
&\qquad=8(-c_{14}+c_{24}-2c_{56}-3c_{23}) \quad \mathrm{IV}
\end{aligned}$$

which are four of nine equations obtained by comparing two expressions for the $p^{(8)}(t)$ polynomial. The remaining five equations are obtained in a similar way.

Similar to (4.36), the magnitude in (4.4) is given by

$$A=\tfrac{1}{16}R(k_1^2+l_1^2+1)(k_2^2+l_2^2+1)(k_3^2+l_3^2+1)(k_4^2+l_4^2+1) \tag{A.2}$$

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Chapter 5

The elastic tensor and eigenvectors of derived 2nd rank tensors

5.1 Introduction

Cowin and Mehrabadi (1987) give a classification of elastic symmetry by means of eigenvectors of 2nd rank tensors connected to the elastic tensor. The method includes the use of eigenvectors of two symmetric 2nd rank tensors derived from the elastic tensor, $C_{ij} = E_{ijkk}$ and $V_{ij} = E_{ikkj}$, (see the review-chapter for details), where E_{ijkl} is the elastic tensor. C_{ij} and V_{ij} are called the "dilatational stiffness tensor" and "Voigt tensor" respectively. C_{ij} contains the elastic stiffnesses relating the stress components to the diagonal components of the strain tensor (dilatational terms). Cowin and Mehrabadi (1987) show that eigenvectors of C_{ij} and V_{ij} are candidates of beeing normal to symmetry planes. In addition, symmetry axes are aligned with eigenvectors of C_{ij} and V_{ij}. Arts (1993) applies this last property in an analysis of estimating a symmetry axis for experimental tensors.

Representation of the elastic tensor by harmonic tensors introduces additional symmetric 2nd rank tensors derived from the elastic tensor.

In the following a hierarchically symmetric tensor (of rank 4) is considered. The definition of this hierarchically symmetric tensor (HST) is identical to the definition of an elastic tensor, except that the stability conditions need not be satisfied for the hierarchically symmetric tensor.

The 2nd rank tensors defined in the decomposition of the HST given by Backus (1970) are denoted by H_{ij}, h_{ij} and t_{ij}. The eigenvectors of those tensors are closely related to symmetry elements of HST. One of the 2nd rank tensors is treated in Backus (1970) and in (Ch. 2). In the following an analysis of several 2nd rank tensors derived from HST, with respect to eigenvalue problems, is presented.

5.2 Eigenvectors of a matrix and the deviatoric part

Lemma.
Let λ be an eigenvalue of a matrix $\mathbf{A}$. Then $\vec{v}$ is an eigenvector of $(\mathbf{A} - k\mathbf{I})$ if and only if $\vec{v}$ is an eigenvector of $\mathbf{A}$. k is any scalar such that $(\mathbf{A} - k\mathbf{I})$ does not vanish, and $\mathbf{I}$ is the identity matrix. The corresponding eigenvalue of $(\mathbf{A} - k\mathbf{I})$ is $\lambda - k$.
Proof:
Assume λ is an eigenvalue of $\mathbf{A}$, and $\vec{v}$ is the corresponding eigenvector, i.e.

$$\mathbf{A}\vec{v} = \lambda\vec{v} \tag{5.1}$$

We then have

$$\begin{aligned} \mathbf{A}\vec{v} = \lambda\vec{v} \quad &\Leftrightarrow \quad \mathbf{A}\vec{v} - k\mathbf{I}\vec{v} = \lambda\vec{v} - k\mathbf{I}\vec{v} \\ &\Leftrightarrow \quad (\mathbf{A} - k\mathbf{I})\vec{v} = (\lambda - k)\vec{v} \end{aligned} \tag{5.2}$$

Thus $(\lambda - k)$ is an eigenvalue of $(\mathbf{A} - k\mathbf{I})$ and $\vec{v}$ is the corresponding eigenvector of $(\mathbf{A} - k\mathbf{I})$.

Assume $\mathbf{A}$ is a 3×3 matrix, $\mathbf{I}$ is the 3×3 identity matrix, and tr$\mathbf{A}$ is the trace of $\mathbf{A}$. If $k = \frac{1}{3}\mathrm{tr}\,\mathbf{A}$, the deviatoric part of $\mathbf{A}$, $\hat{\mathbf{A}} = \mathbf{A} - \frac{1}{3}\mathbf{I}\,\mathrm{tr}\mathbf{A}$ thus has the same eigenvectors as $\mathbf{A}$. The eigenvalues of $\hat{\mathbf{A}}$ are equal to the eigenvalues of $\mathbf{A}$ reduced by $\frac{1}{3}$ tr$\mathbf{A}$.

5.3 Eigenvalues, eigenvectors and invariants of real symmetric 3×3 matrices.

In the following is a review of some algebraic results about eigenvalues and eigenvectors of 3×3 real symmetric matrices. For references see e.g. Boyce and DiPrima (1977), Gantmacher (1960), Kreysig (1988), and Spencer (1980).

Suppose we have a real $n \times n$ symmetric matrix. The eigenvalues and eigenvectors have the following properties:
- All eigenvalues are real, and there always exists a full set of n independent eigenvectors.
- Eigenvectors corresponding to distinct eigenvalues are orthogonal, and establish a set of linear independent unit vectors. See e.g Spencer (1980).
- To a single eigenvalue corresponds a unique eigenvector, except for magnitude. To a multiple eigenvalue with multiplicity m, it is possible to select sets of m mutual orthogonal eigenvectors.
- When all eigenvalues are equal, every set of n orthogonal vectors are eigenvectors and the matrix is a diagonal matrix.

The vector space spanned by eigenvectors corresponding to an eigenvalue is often called the eigenspace of that eigenvalue.

Invariance of eigenvectors relative to symmetry axis.
If a matrix is a representation of a tensor, the eigenvectors have a physical meaning. The orientation of an eigenvector relative to a symmetry axis is independent of the coordinate system. It is also easy to show this independence analytically.
Assume $\mathbf{A}$ is a 3×3 matrix representing a 2nd rank tensor referred to the coordinate system with base vectors $\vec{e}^{(i)}$. $\mathbf{I}$ is the 3×3 diagonal matrix, λ is an eigenvalue of $\mathbf{A}$, and $\vec{v}$ is the corresponding eigenvector. Then we have

$$\mathbf{A}\vec{v} = \lambda\vec{v} \tag{5.3}$$

Let $\tilde{\mathbf{A}}$ represents the tensor in a rotated coordinate system $\tilde{\vec{e}}^{(i)}$ and let $\mathbf{M}$ be the orthonormal transformation representing the rotation. We then have $\tilde{\mathbf{A}} = \mathbf{MAM}^T$. With index notation, this can be written as $\tilde{A}_{ij} = M_{ip}A_{pq}M_{jq} = M_{ip}M_{jq}A_{pq}$. Similarly we have $\tilde{\vec{a}} = \mathbf{M}\vec{a}$ and $\vec{a} = \mathbf{M}^T\tilde{\vec{a}}$ where $\vec{a}$ and $\tilde{\vec{a}}$ are representations of a vector in the two coordinate systems. From (5.3) we have the following:

$$\mathbf{MA}\vec{v} = \lambda\mathbf{M}\vec{v}$$
$$\mathbf{MAM}^T\tilde{\vec{v}} = \lambda\mathbf{MM}^T\tilde{\vec{v}}$$

where $\tilde{\vec{v}}$ is the vector $\vec{v}$ referred to the the new coordinate system. Further we have

$$\tilde{\mathbf{A}}\tilde{\vec{v}} = \lambda\tilde{\vec{v}} \tag{5.4}$$

which shows that $\vec{v}$ referred to the the new coordinate system is the eigenvector of $\tilde{\mathbf{A}}$. This means that relative to a specific coordinate system, a specific eigenvector of a tensor is fixed irrespective of which coordinate system the tensor is referred to. However the components of the eigenvector depend on the chosen reference system. Thus relative to any axis, including a symmetry axis of a medium, an eigenvector of the corresponding tensor is "fixed". The orientation relative to the symmetry axis is independent of the coordinate system the tensor is referred to.

5.4 Tensors generated by the hierarchically symmetric tensor

$C_{ij}, V_{ij}, \hat{C}_{ij}$ and $\hat{V}_{ij}$.

The dilatational modulus tensor C_{ij} and Voigt tensor V_{ij}, respectively, defined in the introduction, are given as:

$$C_{ij} = E_{ijkk} = \begin{pmatrix} c_{11}+c_{12}+c_{13} & c_{16}+c_{26}+c_{36} & c_{15}+c_{25}+c_{35} \\ & c_{12}+c_{22}+c_{23} & c_{14}+c_{24}+c_{34} \\ & & c_{13}+c_{23}+c_{33} \end{pmatrix} \tag{5.5}$$

$$V_{ij} = E_{ikkj} = \begin{pmatrix} c_{11}+c_{55}+c_{66} & c_{16}+c_{26}+c_{45} & c_{15}+c_{46}+c_{35} \\ & c_{22}+c_{44}+c_{66} & c_{24}+c_{34}+c_{56} \\ & & c_{33}+c_{44}+c_{55} \end{pmatrix} \tag{5.6}$$

The off-diagonal components of $\hat{C}_{ij}$ and $\hat{V}_{ij}$ are equal to those of C_{ij} and V_{ij}, respectively. The diagonal elements are:

$$\begin{aligned} \hat{C}_{11} &= \frac{2}{3}(c_{11}-c_{23}) - \frac{1}{3}(c_{22}+c_{33}-c_{12}-c_{13}) \\ \hat{C}_{22} &= \frac{2}{3}(c_{22}-c_{13}) - \frac{1}{3}(c_{11}+c_{33}-c_{12}-c_{23}) \\ \hat{C}_{33} &= \frac{2}{3}(c_{33}-c_{12}) - \frac{1}{3}(c_{11}+c_{22}-c_{13}-c_{23}) \end{aligned} \tag{5.7}$$

and

$$\begin{aligned} \hat{V}_{11} &= \frac{2}{3}(c_{11}-c_{44}) - \frac{1}{3}(c_{22}+c_{33}-c_{55}-c_{66}) \\ \hat{V}_{22} &= \frac{2}{3}(c_{22}-c_{55}) - \frac{1}{3}(c_{11}+c_{33}-c_{44}-c_{66}) \\ \hat{V}_{33} &= \frac{2}{3}(c_{33}-c_{66}) - \frac{1}{3}(c_{11}+c_{22}-c_{44}-c_{55}). \end{aligned} \tag{5.8}$$

From the lemma in section 2, the eigenvectors of C_{ij} and V_{ij} are common to the eigenvectors of the deviatoric parts $\hat{C}_{ij}$ and $\hat{V}_{ij}$ of the two tensors, respectively.

$\underline{H_{ij}, h_{ij} \text{ and } t_{ij}}$.

In the decomposition of the hierarchically symmetric tensor in harmonic tensors, the tensor is first separated into a totally symmetric part and the remainder, a non-totally symmetric part. In a totally symmetric tensor all tensor components with the same unordered indices are identical, regardless of the permutation of the indices. The 2nd rank harmonic tensor in the decomposition of the totally symmetric part of the hierarchically symmetric tensor H_{ij} is given by (see eq. (2.28) Ch. 2):

$$H_{ij} = \frac{1}{21}(\hat{C}_{ij} + 2\hat{V}_{ij}) \tag{5.9}$$

By applying eqs. (5.5), (5.6), (5.7) and (5.8), H_{ij} is expressed in terms of the stiffnesses as:

$$\begin{aligned} H_{11} &= \frac{1}{21}[2c_{11} - c_{22} - c_{33} + \frac{1}{3}(-4c_{44} + 2c_{55} + 2c_{66} + c_{12} + c_{13} - 2c_{23})] \\ H_{22} &= \frac{1}{21}[-c_{11} + 2c_{22} - c_{33} + \frac{1}{3}(2c_{44} - 4c_{55} + 2c_{66} + c_{12} - 2c_{13} + c_{23})] \end{aligned}$$

$$H_{33} = \frac{1}{21}[-c_{11} - c_{22} + 2c_{33} + \frac{1}{3}(2c_{44} + 2c_{55} - 4c_{66} - 2c_{12} + c_{13} + c_{23})]$$

$$H_{12} = \frac{1}{21}(3c_{16} + 3c_{26} + c_{36} + 2c_{45})$$

$$H_{13} = \frac{1}{21}(3c_{15} + c_{25} + 3c_{35} + 2c_{46})$$

$$H_{23} = \frac{1}{21}(c_{14} + 3c_{24} + 3c_{34} + 2c_{56}) \tag{5.10}$$

The symmetric 2nd rank tensor t_{ij}, isomorphic to the non- totally symmetric part of the hierarchically symmetric tensor, is decomposed into a harmonic tensor h_{ij} and a scalar h in the following way (see Ch. 2):

$$t_{ij} = h_{ij} + \frac{1}{2}h\delta_{ij}, \tag{5.11}$$

where h_{ij} and h, (see Ch. 2) eqs. (2.33) and (2.32)), are given by:

$$h_{ij} = \frac{2}{3}(\hat{C}_{ij} - \hat{V}_{ij}) \tag{5.12}$$

and

$$h = \frac{1}{9}(\text{tr } C_{ij} - \text{tr } V_{ij}) = \frac{1}{9}(C_{ii} - V_{ii}) = \frac{2}{9}(c_{12} + c_{13} + c_{23} - c_{44} - c_{55} - c_{66}) \tag{5.13}$$

In (5.11), $\frac{1}{2}h$ is a scalar, which means that t_{ij} and h_{ij} have common eigenvectors according to the Lemma in section 2. The trace of t_{ij} is given by

$$\text{tr } t_{ij} = t_{ii} = h_{ii} + \frac{1}{2}h\delta_{ii} = \frac{3}{2}h \tag{5.14}$$

since h_{ij}, as the difference of two traceless tensors, is traceless.
From (5.11) and (5.14) we have

$$h_{ij} = t_{ij} - \frac{1}{3}\text{tr}(t_{ij})\,\delta_{ij}$$

or

$$h_{ij} = \hat{t}_{ij} \tag{5.15}$$

which means that h_{ij} is the deviatoric part of t_{ij}.

From (5.5) and (5.6), we have:

$$\text{tr } C = c_{11} + c_{22} + c_{33} + 2c_{12} + 2c_{13} + 2c_{23}$$

$$\text{tr } V = c_{11} + c_{22} + c_{33} + 2c_{44} + 2c_{55} + 2c_{66}$$

By applying eqs. (5.11), (5.12) and (5.13), t_{ij} is expressed in terms of the stiffnesses as:

$$t_{11} = \frac{1}{3}(c_{44} - c_{55} - c_{66} + c_{12} + c_{13} - c_{23})$$

$$t_{22} = \frac{1}{3}(-c_{44} + c_{55} - c_{66} + c_{12} - c_{13} + c_{23})$$

$$t_{33} = \frac{1}{3}(-c_{44} - c_{55} + c_{66} - c_{12} + c_{13} + c_{23})$$

$$t_{12} = \frac{2}{3}(c_{36} - c_{45})$$

$$t_{13} = \frac{2}{3}(c_{25} - c_{46})$$

$$t_{23} = \frac{2}{3}(c_{14} - c_{56}). \tag{5.16}$$

h_{ij} is expressed by the elastic constants as

$$h_{11} = \frac{2}{9}(2c_{44} - c_{55} - c_{66} + c_{12} + c_{13} - 2c_{23})$$

$$h_{22} = \frac{2}{9}(-c_{44} + 2c_{55} - c_{66} + c_{12} - 2c_{13} + c_{23})$$

$$h_{33} = \frac{2}{9}(-c_{44} - c_{55} + 2c_{66} - 2c_{12} + c_{13} + c_{23})$$

$$h_{12} = \frac{2}{3}(c_{36} - c_{45})$$

$$h_{13} = \frac{2}{3}(c_{25} - c_{46})$$

$$h_{23} = \frac{2}{3}(c_{14} - c_{56}). \tag{5.17}$$

From (5.12) $\mathbf{h} = 2/3(\hat{\mathbf{C}} - \hat{\mathbf{V}})$. The fact that $\mathbf{h}$ is a linear combination of $\hat{\mathbf{C}}$ and $\hat{\mathbf{V}}$ motivates the following consideration:
Generally, suppose a matrix $\mathbf{C}$ is a linear combination of two matrices $\mathbf{A}$ and $\mathbf{B}$. We will show that this is not a sufficient condition for eigenvectors of $\mathbf{A}$ or $\mathbf{B}$ to be eigenvectors of $\mathbf{C}$. Neither is a linear combination of eigenvectors of $\mathbf{A}$ and $\mathbf{B}$ eigenvectors of $\mathbf{C}$. Suppose $\mathbf{C} = a\mathbf{A} + b\mathbf{B}$, where a and b are scalars, and

$$\mathbf{A}\vec{x} = \kappa\vec{x} \qquad\qquad \mathbf{B}\vec{y} = \lambda\vec{y}$$

Thus $\vec{x}$ and $\vec{y}$ are eigenvectors of $\mathbf{A}$ and $\mathbf{B}$ respectively. κ and λ are the eigenvalues. To search for an eigenvector of $\mathbf{C}$ to be on the form $r\vec{x}+s\vec{y}$, where r and s are scalars, try the following calculation:

$$\begin{aligned}\mathbf{C}(r\vec{x} + s\vec{y}) &= (a\mathbf{A} + b\mathbf{B})(r\vec{x} + s\vec{y}) \\ &= ar\kappa\vec{x} + bs\lambda\vec{y} + br\mathbf{B}\vec{x} + as\mathbf{A}\vec{y}\end{aligned} \tag{5.18}$$

which generally is not a multiple of $(r\vec{x} + s\vec{y})$. Thus $(r\vec{x} + s\vec{y})$ is not generally an eigenvector of $\mathbf{C}$, even if $a = 2/3$ and $b = -2/3$ the linear combination above is not

an eigenvector of **C**. In addition, if $r = 0$ or $s = 0$, (5.18) shows that an eigenvector of **A** or of **B** is not generally an eigenvector of the linear combination **C**.
Result:
The fact that h_{ij} is a linear combination of $\hat{C}_{ij}$ and $\hat{V}_{ij}$ is not a sufficient condition for eigenvectors of $\hat{C}_{ij}$ or $\hat{V}_{ij}$ to be eigenvectors of h_{ij}. Neither is a linear combination of eigenvectors of $\hat{C}_{ij}$ or $\hat{V}_{ij}$ eigenvectors of h_{ij}. A similar statement is valid for the harmonic tensor H_{ij}.

Under the condition of non-vanishing tensors, we have the following summary:

Summary:
1. A tensor A_{ij} and its deviatoric part have the same set of eigenvectors.
2. C_{ij} and V_{ij} have the same set of eigenvectors as their deviatoric parts respectively.
3. h_{ij} and t_{ij} have the same set of eigenvectors.
4. Eigenvectors of $\hat{C}_{ij}$ and $\hat{V}_{ij}$, or linear combinations of them, are generally eigenvectors of neither H_{ij} nor h_{ij}.

The question is then if higher symmetry of the corresponding hierarchically symmetric tensor introduces relationships between, or coincidence of, eigenvectors of the 2nd rank tensors **H**, **h**, $\hat{\mathbf{C}}$ and $\hat{\mathbf{V}}$. Let us start with monoclinic symmetry.

Monoclinic symmetry.
For monoclinic symmetry, we have

$$c_{14} = c_{15} = c_{24} = c_{25} = c_{34} = c_{35} = c_{46} = c_{56} = c_{45} = 0$$

with the 3- axis as symmetry axis. c_{36} could be chosen to be zero instead of c_{45}. Thus the tensor of monoclinic symmetry has 12 independent components (see Helbig (1994)).
H_{ij}.
For H_{ij}, the expressions for the diagonal terms are the same as for triclinic symmetry, and we have

$$\begin{aligned}
H_{11} &= \frac{1}{21}[2c_{11} - c_{22} - c_{33} + \frac{1}{3}(-4c_{44} + 2c_{55} + 2c_{66} + c_{12} + c_{13} - 2c_{23})] \\
H_{22} &= \frac{1}{21}[-c_{11} + 2c_{22} - c_{33} + \frac{1}{3}(2c_{44} - 4c_{55} + 2c_{66} + c_{12} - 2c_{13} + c_{23})] \\
H_{33} &= \frac{1}{21}[-c_{11} - c_{22} + 2c_{33} + \frac{1}{3}(2c_{44} + 2c_{55} - 4c_{66} - 2c_{12} + c_{13} + c_{23})] \\
H_{12} &= \frac{1}{21}(3c_{16} + 3c_{26} + c_{36}) \qquad H_{13} = 0 \qquad H_{23} = 0
\end{aligned} \tag{5.19}$$

h_{ij} and t_{ij}.
Since t_{ij} and h_{ij} have identical eigenvectors, we could as well analyse t_{ij} as h_{ij}. t_{ij}

for monoclinic symmetry has the following expression:

$$t_{11} = \frac{1}{3}(c_{44} - c_{55} - c_{66} + c_{12} + c_{13} - c_{23})$$

$$t_{22} = \frac{1}{3}(-c_{44} + c_{55} - c_{66} + c_{12} - c_{13} + c_{23})$$

$$t_{33} = \frac{1}{3}(-c_{44} - c_{55} + c_{66} - c_{12} + c_{13} + c_{23})$$

$$t_{12} = \frac{2}{3}c_{36} \qquad t_{13} = 0 \qquad t_{23} = 0 \tag{5.20}$$

$\underline{\hat{C}_{ij}}$.
From (5.5) and (5.7) $\hat{C}_{ij}$ is given as:

$$\hat{C}_{11} = \frac{2}{3}(c_{11} - c_{23}) - \frac{1}{3}(c_{22} + c_{33} - c_{12} - c_{13})$$

$$\hat{C}_{22} = \frac{2}{3}(c_{22} - c_{13}) - \frac{1}{3}(c_{11} + c_{33} - c_{12} - c_{23})$$

$$\hat{C}_{33} = \frac{2}{3}(c_{33} - c_{12}) - \frac{1}{3}(c_{11} + c_{22} - c_{13} - c_{23})$$

$$\hat{C}_{12} = c_{16} + c_{26} + c_{36} \qquad \hat{C}_{13} = 0 \qquad \hat{C}_{23} = 0 \tag{5.21}$$

$\underline{\hat{V}_{ij}}$.
From (5.6) and (5.8) $\hat{V}_{ij}$ is given as:

$$\hat{V}_{11} = \frac{2}{3}(c_{11} - c_{44}) - \frac{1}{3}(c_{22} + c_{33} - c_{55} - c_{66})$$

$$\hat{V}_{22} = \frac{2}{3}(c_{22} - c_{55}) - \frac{1}{3}(c_{11} + c_{33} - c_{44} - c_{66})$$

$$\hat{V}_{33} = \frac{2}{3}(c_{33} - c_{66}) - \frac{1}{3}(c_{11} + c_{22} - c_{44} - c_{55})$$

$$\hat{V}_{12} = c_{16} + c_{26} \qquad \hat{V}_{13} = 0 \qquad \hat{V}_{23} = 0 \tag{5.22}$$

MATHEMATICA is used in calculating eigenvectors of some of the 2nd rank tensors generated by the hierarchically symmetric tensor. For each of the tensors the eigenvalues are different.

$\underline{t_{ij}}$.
The eigenvectors of t_{ij} for monoclinic symmetry is:

$$\vec{e_1}^{(t)} = [1, \frac{-c_{13} + c_{23} - c_{44} + c_{55} - \sqrt{R^{(t)}}}{2c_{36}}, 0]$$

$$\vec{e_2}^{(t)} = [1, \frac{-c_{13} + c_{23} - c_{44} + c_{55}) + \sqrt{R^{(t)}}}{2c_{36}}, 0]$$

$$\vec{e_3}^{(t)} = [0, 0, 1]$$

where $R^{(t)}$ is given as

$$R^{(t)} = c_{13}^2 - 2c_{13}c_{23} + c_{23}^2 + 4c_{36}^2 + 2c_{13}c_{44} - 2c_{23}c_{44} + c_{44}^2 - 2c_{13}c_{55} + 2c_{23}c_{55} - 2c_{44}c_{55} + c_{55}^2$$

and can be expressed as

$$R^{(t)} = c_{44}^2 + c_{55}^2 - 2c_{44}c_{55} + 4c_{36}^2 + (c_{13} - c_{23} + 2c_{44} - 2c_{55})(c_{13} - c_{23})$$

or

$$R^{(t)} = c_{44}^2 + c_{55}^2 - 2c_{44}c_{55} + 4c_{36}^2 + (c_{13} - c_{23})^2 + 2(c_{44} - c_{55})(c_{13} - c_{23})$$

$\underline{\hat{C}_{ij}}$

The eigenvectors of $\hat{C}_{ij}$ are:

$$\vec{e_1}^{(C)} = [1, \frac{-c_{11} + c_{22} - c_{13} + c_{23} - \sqrt{R^{(C)}}}{2(c_{16} + c_{26} + c_{36})}, 0]$$

$$\vec{e_2}^{(C)} = [1, \frac{-c_{11} + c_{22} - c_{13} + c_{23} + \sqrt{R^{(C)}}}{2(c_{16} + c_{26} + c_{36})}, 0]$$

$$\vec{e_3}^{(C)} = [0, 0, 1]$$

where $R^{(C)}$ is given as

$$R^{(C)} = c_{11}^2 + 2c_{11}c_{13} + c_{13}^2 + 4c_{16}^2 - 2c_{11}c_{22} - 2c_{13}c_{22} + c_{22}^2 - 2c_{11}c_{23}$$
$$-2c_{13}c_{23} + 2c_{22}c_{23} + c_{23}^2 + 8c_{16}c_{26} + 4c_{26}^2 + 8c_{16}c_{36} + 8c_{26}c_{36} + 4c_{36}^2$$

and can be expressed as

$$R^{(C)} = c_{11}^2 + c_{22}^2 - 2c_{11}c_{22} + (c_{13} - c_{23})^2$$
$$+2(c_{11} - c_{22})(c_{13} - c_{23}) + 4(c_{16} + c_{26} + c_{36})^2$$

$\underline{\hat{V}_{ij}}$

The eigenvectors of $\hat{V}_{ij}$ are:

$$\vec{e_1}^{(V)} = [1, \frac{-c_{11} + c_{22} + c_{44} - c_{55} - \sqrt{R^{(V)}}}{2(c_{16} + c_{26})}, 0]$$

$$\vec{e_2}^{(V)} = [1, \frac{-c_{11} + c_{22} + c_{44} - c_{55} + \sqrt{R^{(V)}}}{2(c_{16} + c_{26})}, 0]$$

$$\vec{e_3}^{(V)} = [0, 0, 1]$$

where $R^{(V)}$ is given as

$$R^{(V)} = c_{11}^2 + 4c_{16}^2 - 2c_{11}c_{22} + c_{22}^2 + 8c_{16}c_{26} + 4c_{26}^2 - 2c_{11}c_{44} + 2c_{22}c_{44} + c_{44}^2 + 2c_{11}c_{55} - 2c_{22}c_{55} - 2c_{44}c_{55} + c_{55}^2$$

or

$$R^{(V)} = c_{11}^2 + c_{22}^2 + 4(c_{16} + c_{26})^2 + 2(c_{44} - c_{55})(c_{22} - c_{11}) + (c_{44} - c_{55})^2$$

The analysis so far show that $t_{ij}, \hat{C}_{ij}$ and $\hat{V}_{ij}$ do not generally have the same set of eigenvectors. Further algebraic manipulations would not change that, since the eigenvectors in each case are expressed by means of different sets of elastic constants. However the symmetry axis is a common eigenvector.

From (5.10) it is seen that the expressions for H_{ij} is rather complicated, and so is the expressions for the eigenvectors calculated by MATHEMATHICA. Since H_{ij} is expressed my means of a set of elastic constants different from each of the sets in the three cases analysed above, it is reasonable to think that the set of eigenvectors of H_{ij} do not coincide with the eigenvectors of any of the sets analysed. However the symmetry axis is one of the eigenvectors. To prove that no two of the four 2nd rank tensors under consideration generally have identical sets of eigenvectors, it is sufficient to give a counterexample of coincident sets of eigenvectors. That is given in the following:

The following monoclinic tensor $m_{\alpha\beta}$ is given:

$$m_{\alpha\beta} = \begin{pmatrix} 7.006 & -0.001 & 2.296 & 0.000 & 0.000 & -0.062 \\ & 2.796 & -1.796 & 0.000 & 0.000 & -0.076 \\ & & 6.650 & 0.000 & 0.000 & -1.541 \\ & & & 1.725 & 0.000 & 0.000 \\ & & & & 3.425 & 0.000 \\ & & & & & 0.499 \end{pmatrix} \tag{5.23}$$

The symmetry axis is the 3-axis, and $c_{45} = 0$. This tensor is the same as the monoclinic tensor in Ch. 2, where the tensor is represented in a rotated coordinate systems. There are three different eigenvalues for each of the derived 2nd rank tensors. The eigenvectors for each of C_{ij}, $\hat{C}_{ij}$, $\hat{V}_{ij}$, t_{ij} and H_{ij}, given by MATHEMATICA, are respectively:

$$\begin{aligned} C_{ij}: &\quad \{(0.1946, 1, 0), (-5.1392, 1, 0), (0, 0, 1)\}, \\ \hat{C}_{ij}: &\quad \{(0.1946, 1, 0), (-5.1392, 1, 0), (0, 0, 1)\}, \\ \hat{V}_{ij}: &\quad \{(0.0233, 1, 0), (-42.8494, 1, 0), (0, 0, 1)\}, \\ t_{ij}: &\quad \{(0.4897, 1, 0), (-2.0420, 1, 0), (0, 0, 1)\}, \\ H_{ij}: &\quad \{(0.0963, 1, 0), (-10.3888, 1, 0), (0, 0, 1)\}. \end{aligned} \tag{5.24}$$

Since the eigenvalues are distinct, the eigenvectors are unique except for the magnitude. Notice that C_{ij} and $\hat{C}_{ij}$ have equal eigenvectors. One eigenvector is common for the five tensors, namely the symmetry axis (here (0, 0, 1)).

If the eigenvectors have any physical meaning, they are related to the symmetry, and not to the coordinate system. If e.g. the monoclinic tensor is given relative to a coordinate system different from the symmetry coordinate system, all the four 2nd rank tensors analysed have one eigenvector parallel to the symmetry axis.
Conclusion: All seven 2nd rank tensors under consideration have the symmetry axis as one of the eigenvectors. There are four 2nd rank tensors with different sets of eigenvectors.

Orthorhombic symmetry.
For orthorhombic symmetry, we have in the symmetry coordinate system:

$$c_{14} = c_{15} = c_{16} = c_{24} = c_{25} = c_{26} = c_{34} = c_{35} = c_{36} = c_{45} = c_{46} = c_{56} = 0$$

The only difference between orthorhombic and monoclinic symmetry with respect to the 2nd rank tensors under consideration is that for orthorhombic symmetry all three off-diagonal components vanish. For each of the 2nd rank tensors, the diagonal elements are different. Since the off-diagonal elements vanish, the diagonal elements are the eigenvalues. Since they are different, each of the tensors have only one set of eigenvectors. The eigenvectors are the symmetry axes. The eigenvalues are invariant against orthogonal transformation, and thus against any rotation of reference coordinate system. Note that in any coordinate system then each of the tensors have only one set of eigenvectors, and they coincide with the symmetry axes.

Tetragonal symmetry.
With the 3-axis as symmetry axis, the following elastic constants vanish:

$$c_{14},\ c_{15},\ c_{24},\ c_{25},\ c_{34},\ c_{35},\ c_{36},\ c_{45},\ c_{46},\ c_{56},$$

and there are the following relations between elastic constants:

$$c_{22} = c_{11}, \quad c_{23} = c_{13}, \quad c_{26} = -c_{16} \text{ and } c_{55} = c_{44}.$$

In addition, the coordinate system can be rotated to remove c_{16} and c_{26}. The tensor has six independent components, and has the same symmetry as the traditional tetragonal (7) (se Helbig (1994)).
Two common properties for the four 2nd rank tensors $H_{ij}, t_{ij}, \hat{C}_{ij}$ and $\hat{V}_{ij}$ are the following:

1. The off-diagonal components are identically zero.

2. The $(1,1)$- and the $(2,2)$ components are equal for each of the four tensors. That means that there are one single eigenvalue and one with multiplicity two. Thus the 3- axis are unique, while any set of two vectors in the (1,2)- plane are eigenvectors.

Here there are a set of indefinitly many eigenvectors in the plane perpendicular to the 3- axis, and, according to Cowin and Mehrabadi (1987), only four eigenvectors of the set are normals to plane of symmetry. The same properties also hold for h_{ij}, C_{ij} and V_{ij}.

Hexagonal symmetry (transverse isotropy).
In addition to the restrictions on the elastic constants for tetragonal symmetry, there are the following for hexagonal symmetry, in all coordinate systems with the 3- axis as symmetry axis:

$$c_{16} = c_{26} = 0 \quad \text{and} \quad c_{66} = \frac{1}{2}(c_{11} - c_{12})$$

There are the following properties for the four 2nd rank tensors $H_{ij}, t_{ij}, \hat{C}_{ij}$ and $\hat{V}_{ij}$:

1. All off-diagonal components are expressed by the elastic constants which vanish (for all rotations around the 3- axis).
2. The $(1,1)$- and the $(2,2)$ components are equal for each of the four tensors. That means that the 3- axis are unique, while any set of two vectors in the (1,2)- plane are eigenvectors.

The same properties also hold for h_{ij}, C_{ij} and V_{ij}. Se an example later.

Cubic symmetry.
For cubic symmetry, there are three independent elastic constants, and we have the following relations between the non-vanishing constants:

$$c_{22} = c_{33} = c_{11}, \quad c_{13} = c_{23} = c_{12} \quad \text{and} \quad c_{44} = c_{55} = c_{66}.$$

In this case, four of the 2nd rank tensors vanish. The norm of those tensors is zero, and thus the norm is zero in all coordinate systems. The tensor vanish in all coordinate systems. We have the following properties for the 2nd rank tensors considered:

1. $\hat{C}_{ij}, \hat{V}_{ij}, H_{ij},$ and h_{ij} vanish, i.e. all deviatoric 2nd rank tensors in addition to H_{ij} vanish. (h_{ij} is the deviatoric part of t_{ij}).
2. All off-diagonal components for the remaining 2nd rank tensors vanish. The non-vanishing tensors are: C_{ij}, V_{ij} and t_{ij}.
3. All tensor components are equal, this means identical eigenvalues, and all vectors are eigenvectors.

Isotropic symmetry.
For isotropic symmetry, there are two independent elastic constants, and the following relations between the non-vanishing constants:

$$c_{22} = c_{33} = c_{11}, \quad c_{13} = c_{23} = c_{12} \quad \text{and} \quad c_{44} = c_{55} = c_{66} = \frac{1}{2}(c_{11} - c_{12}).$$

The conclusion is the same as for cubic symmetry. Four deviatoric 2nd rank tensors vanish. We have the following properties for the 2nd rank tensors considered:

1. $\hat{C}_{ij}$, $\hat{V}_{ij}$, H_{ij} and h_{ij} vanish.

2. All off-diagonal components for the remaining 2nd rank tensors vanish. The non-vanishing tensors are: C_{ij}, V_{ij} and t_{ij}.

3. All tensor components are equal, this means identical eigenvalues, and all vectors are eigenvectors.

Trigonal symmetry .
In addition to the conditions on the elastic coefficients for hexagonal symmetry, there are the following:

$$c_{24} = -c_{14} = -c_{56}, \quad \text{and} \quad c_{25} = c_{46} = -c_{15}.$$

This is overwriting conditions from hexagonal symmetry. c_{15}, c_{25} and c_{46} can be removed by a rotation about the 3- axis. Thus there are at most six independent elastic coefficients (Helbig (1994)).

In this case we have the same conclusion as for tetragonal symmetry. The properties for the four 2nd rank tensors $H_{ij}, t_{ij}, \hat{C}_{ij}$ and $\hat{V}_{ij}$ are the following:

1. The off-diagonal components are identically zero.

2. The $(1,1)$ and the $(2,2)$ components are equal for each of the four tensors. That means that the 3- axis are unique, while any set of two vectors in the (1,2)- plane are eigenvectors.

Example. Eigenvectors for higher symmetry.

Even for higher symmetry than orthorhombic symmetry, the calculated eigenvectors for the different 2nd rank tensors do not necessarily coincide since there are infinitly many eigenvectors. However, eigenvectors are always aligned with symmetry axes.

As an example, let us concider a tensor of hexagonal symmetry and calculate the eigenvectors. In a symmetry coordinate system the tensor is given as:

$$m_{\alpha\beta}^{(hex)} = \begin{pmatrix} 3.150 & 1.950 & 1.850 & 0.000 & 0.000 & 0.000 \\ & 3.150 & 1.850 & 0.000 & 0.000 & 0.000 \\ & & 6.650 & 0.000 & 0.000 & 0.000 \\ & & & 2.550 & 0.000 & 0.000 \\ & & & & 2.550 & 0.000 \\ & & & & & 0.600 \end{pmatrix} \tag{5.25}$$

and in a specific rotated coordinate system the same tensor is represented as:

$$m_{\alpha\beta}^{(hexr)} = \begin{pmatrix} 4.147 & 1.521 & 1.765 & -0.266 & 0.607 & 0.945 \\ & 6.254 & 1.241 & 0.511 & -0.489 & 0.385 \\ & & 4.796 & 1.082 & 0.523 & -0.331 \\ & & & 1.649 & 0.271 & -0.102 \\ & & & & 1.220 & 0.533 \\ & & & & & 1.708 \end{pmatrix}. \quad (5.26)$$

To illustrate some of the properties discussed in this section, and to show that only one eigenvector is common and unique for different 2nd rank tensors, the eigenvectors of C_{ij}, $\hat{C}_{ij}$, V_{ij} and H_{ij} are calculated. MATHEMATICA is used in the calculations. The calculated orthonormal eigenvectors are shown in Table 5.1. From the table we see that there is an eigenvector which is common to all the tensors, as expected. From the theory one eigenvector is unique, namely one parallel to the symmetry axis. C_{ij}, $\hat{C}_{ij}$ have coincident eigenvectors. However any two eigenvectors from one of those two tensors perpendicular to the symmetry axis might be different from eigenvectors of the other tensor since any vector perpendicular to the symmetry axis is an eigenvector for hexagonal symmetry. The computer routine calculated a common set of three eigenvectors for C_{ij} and the deviatoric part $\hat{C}_{ij}$. Only for monoclinic and triclinic symmetry a tensor and its deviatoric part always have a unique common set of three eigenvectors.

For each of the four tensors, different eigenvectors are calculated in the plane perpendicular to the symmetry axis. From the theory, all vectors in the plane perpendicular to the symmetry axis are eigenvectors.

Tensor	*Eigenvectors*
C	[−0.377, −0.779, −0.501], [−0.780, −0.024, 0.625], [0.499, −0.626, 0.599].
$\hat{C}$	[−0.377, −0.779, −0.501], [−0.780, −0.024, 0.625], [0.499, −0.626, 0.599].
V	[−0.377, −0.779, −0.501], [−0.926, 0.327, 0.189], [−0.017, −0.535, 0.845].
H	[−0.377, −0.779, −0.501], [0.183, −0.592, 0.784], [−0.908, 0.204, 0.366].

Table 5.1: Normalised eigenvectors for C_{ij}, $\hat{C}_{ij}$, V_{ij} and H_{ij} for hexagonal symmetry.

In Arts (1993) we have the following: " $\cdots$ for media of orthotropic or higher symmetry the eigenvectors of C_{ij} and V_{ij} are identical and aligned with the crystallographic directions $\cdots$". We have seen that for hexagonal symmetry, there are infinitely many eigenvectors in one of the symmetry planes. They are all normals to symmetry planes. In this case the set of eigenvectors for the two tensors are identical, although the three eigenvectors for each of the tensors need not be identical. For tetragonal symmetry, there are indefinitly many eigenvectors as well, but there are neither indefinitely many symmetry planes, nor indefinitely many symmetry axes. For cubic symmetry all directions are eigenvectors. Which crystallographic directions are they aligned with?

Table 5.2 shows a summary of the analysis. The number of independent elastic coefficients is given in the left column in the table. The reference for the numbers are Helbig (1994).

Symmetry	C_{ij}	$\hat{C}_{ij}$	V_{ij}	$\hat{V}_{ij}$	H_{ij}	t_{ij}	h_{ij}
Tri– triclinic (18)	3 axes	Same as for C_{ij}	3 axes	Same as for V_{ij}	3 axes	3 axes	Same as for t_{ij}
Mono– clinic (12)	Symm.– axis. 2 unique axes ⊥ symm.– axis.	Same as for C_{ij}.	Symm.– axis. 2 unique axes ⊥ symm.– axis.	Same as for V_{ij}.	Symm.– axis. 2 unoque axes ⊥ symm.– axis.	Symm.– axis. 2 unique axes ⊥ symm.– axis.	Same as for t_{ij}
Ortho– rhombic (9)	3 symm.– axes.	Same as for C_{ij}	Same as for. C_{ij}	Same as for C_{ij}	Same as for. C_{ij}	Same as for. Cij	Same as for C_{ij}
Tri– gonal (6)	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm. axis Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.
Tetra– gonal (6)	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm. axix Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis Any 2 axes ⊥ symm.– axis.
Hexa– gonal (5)	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm. axix Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis. Any 2 axes ⊥ symm.– axis.	Symm.– axis Any 2 axes ⊥ symm.– axis.
Cubic (3)	Any vector.	Tensor vanish.	Any vector.	Tensor vanish.	Tensor vanish.	Any vector.	Tensor vanish
Isotropic (2)	Any vector.	Tensor vanish.	Any vector.	Tensor vanish.	Tensor vanish.	Any vector.	Tensor vanish.

⊥ : perpendicular to. Symm.: symmetry. The numbers in the first column is the number of independent elastic components.

Table 5.2: Eigenvectors for different 2nd rank tensors for different symmetry. It is also marked when specific tensors vanish.

5.5 Conclusion

The seven analysed 2nd rank tensors derived from the hierarchically symmetric tensor give four different eigenvalue problems in the determination of different sets of eigenvectors. The deviatoric part of a tensor does not have eigenvectors which are not eigenvectors of the tensor itself.

Except for the magnitude, each of of the four eigenvalue problems give three unique eigenvectors for triclinic and monoclinic symmetry. For monoclinic and higher symmetry, there exist always eigenvectors aligned with symmetry axes and normals to symmetry planes.

For tetragonal, trigonal and hexagonal symmetry, any vector normal to the symmetry axis is an eigenvector.

For cubic- and isotropic symmetry, the diagonal components of each of the 2nd rank tensors are identical, and the off-diagonal components vanish. The eigenvalues have multiplicity three, and any vector is an eigenvector. Since the diagonal components are identical in the 2nd rank diagonal matrices, the deviatoric part vanish for each of the tensors. The deviatoric 2nd rank tensors concidered here are $\hat{C}_{ij}$, $\hat{V}_{ij}$ and h_{ij}. Since H_{ij} is a linear combination of $\hat{C}_{ij}$ and $\hat{V}_{ij}$, H_{ij} vanish when $\hat{C}_{ij}$ and $\hat{V}_{ij}$ vanish. The 2nd rank tensors which do not vanish for cubic and isotropic symmetry, are C_{ij}, V_{ij} and t_{ij}.

When the symmetry is close to ideal symmetry, it is reasonable to think that one of the eigenvectors from each of the 2nd rank tensors is close to the symmetry axis. Averaging could then give an estimate of the approximation of the direction of a symmetry axis, (see Arts, Helbig and Rasolofosaon (1991) and Arts (1993)).

For real media, all elastic tensors are triclinic, and the four tensors C_{ij}, V_{ij}, H_{ij} and t_{ij} is suggested in searching for symmetry axes.

Since $\hat{C}_{ij}, \hat{V}_{ij}, H_{ij}$ and t_{ij} vanish for cubic and isotropic symmetry, further development is suggested to see if those tensors might become a tool in defining a degree of deviation from isotropic symmetry.

Chapter 6

Sensitivity of Maxwell multipoles by perturbation of the hierarchically symmetric tensor

6.1 Introduction

A geometric picture of the hierarchically symmetric tensor (HST) is given by bouquets of three-dimensional vectors defining Maxwell multipoles. The theoretical foundation was presented by Backus (1970), and is further developed and applied in chapters 2 and 4. The directions defined by Maxwell multipoles are here called space directions. Hierarchically symmetric tensors C_{ijkl} are defined as fourth rank tensors in three dimensions, satisfying the symmetry conditions $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$.

In two-index notation, HST can be represented by a symmetric 6×6 matrix as

$$c_{\alpha\beta} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ & & c_{33} & c_{34} & c_{35} & c_{36} \\ & & & c_{44} & c_{45} & c_{46} \\ & & & & c_{55} & c_{56} \\ & & & & & c_{66} \end{pmatrix} \tag{6.1}$$

A classification of higher symmetry classes by means of the bouquets of space directions in Maxwell multipoles is given in Ch. 4. The bouquets exhibit exactly the same symmetry as the HST. The difference is that this symmetry is open to inspection in 3- dimensional space irrespective of orientation of the coordinate system. In addition formulas for the magnitude of the vectors are developed. The analysis is based on decomposition of the hierarchically symmetric tensor by five harmonic tensors, namely one fourth rank tensor, two 2nd rank tensors and two scalars (see Backus (1970)). Harmonic tensors are defined as totally symmetric and traceless tensors. In a totally symmetric tensor all tensor components with a specific set of indices are equal, regardless of the permutation of the indices. A tensor is traceless when the contraction over all pairs of two indices is zero. See further discussion in Cp. 4.

If a real elastic medium is said to have higher symmetry than triclinic, the symmetry is always an approximation to exact symmetry. In addition, although a medium has some specific symmetry, as for instance transverse isotropic or orthorhombic, the corresponding experimentally determined elastic tensor is never an ideal tensor in the sense that it is a member of the group of tensors specifying a symmetry class. Thus, in an anisotropic material the elastic tensor generally has 21 non-vanishing components. The theoretical work in the previous chapters, so far has considered tensors with ideal symmetry.

In the following, perturbation of tensors of ideal symmetry is analysed as a model for real media. The influence on Maxwell multipoles of perturbing tensors of ideal symmetry is the main topic of the investigation.

6.2 Review of Maxwell multipoles for harmonic tensors

Harmonic tensors of rank q are isomorphic to homogeneous polynomials of degree q, where the polynomial is expressed by the coefficients of the hierarchically symmetric tensor. The components of Maxwell multipoles are determined from the harmonic polynomials in the following way:
- A homogeneous polynomial in three variables of degree q, $P^{(q)}(x,y,z)$, is mapped on a homogeneous polynomial of degree $2q$ with complex coefficients in two variables.
- A homogeneous polynomial of degree $2q$ in two variables is mapped on an inhomogeneous polynomial of degree $2q$ in one variable ($P^{(2q)}(t)$). The roots of these polynomials are directly related to the components of the Maxwell multipoles.

Let $z = k + il$ be a root of $P^{(2q)}(t)$. The space direction $\mathbf{v}$ are given by a normalization of the vector $x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$ given as:

$$x = -k \qquad y = -l \qquad z = \frac{1}{2}(k^2 + l^2 - 1) \tag{6.2}$$

If θ is the angle between $\mathbf{v}$ and the z -axis, θ is given as

$$\theta = \arctan \frac{2(k^2 + l^2)^{1/2}}{k^2 + l^2 - 1}$$

or

$$\theta = \arctan \frac{2|z|}{|z|^2 - 1} \tag{6.3}$$

where $|z| = (k^2 + l^2)^{1/2}$ is the length of z.

6.2.1 The fourth rank harmonic tensor H_{ijkl}

The hierarchically symmetric tensor is decomposed by five harmonic tensors, namely one fourth rank tensor, two 2nd rank tensors and two scalars. The forth rank harmonic tensor is isomorphic to a homogeneous polynomial of degree four in three variables, and each of the two 2nd rank tensors is isomorphic to a homogeneous polynomial of degree two. Because of the totally symmetry of H_{ijkl}, we have

$$H_{2323} = H_{2233}, \quad H_{2313} = H_{3312}, \quad H_{2312} = H_{2213},$$

$$H_{1313} = H_{1133}, \quad H_{1312} = H_{1123}, \quad \text{and} \quad H_{1212} = H_{1122} \tag{6.4}$$

The fourth rank harmonic tensor, H_{ijkl}, thus can be represented by a symmetric 6×6 matrix as:

$$H_{ijkl} = \begin{pmatrix} H_{1111} & H_{1122} & H_{1133} & H_{1123} & H_{1113} & H_{1112} \\ & H_{2222} & H_{2233} & H_{2223} & H_{2213} & H_{2212} \\ & & H_{3333} & H_{3323} & H_{3313} & H_{3312} \\ & & & (H_{2233}) & (H_{3312}) & (H_{2213}) \\ & & & & (H_{1133}) & (H_{1123}) \\ & & & & & (H_{1122}) \end{pmatrix}, \tag{6.5}$$

Each component in paranthesis is identical to one of the components in the upper three rows in the matrix. Thus H_{ijkl} has 15 distinct components. The number of independent components is further reduced by six, since the six traces are identically zero (the traces are: $H_{iikl}, H_{ijil}, H_{ijki}, H_{ijjl}, H_{ijkj}$ and H_{ijkk}). H_{ijkl} thus has nine independent components.

The following mapping of the fourth rank harmonic tensor H_{ijkl} on a 8th degree polynomial in one variable is presented in Ch. 4. The 4th degree homogeneous polynomial generated by the harmonic tensor H_{ijkl} and the corresponding 8th degree polynomial in t are given, respectively, as:

$$P^{(4)}(x, y, z) = H_{1111}x^4 + 4H_{1112}x^3y + 4H_{1113}x^3z$$

$$+6H_{1122}x^2y^2 + 12H_{1123}x^2yz + 6H_{1133}x^2z^2 + 4H_{1222}xy^3$$

$$+12H_{1223}xy^2z + 12H_{1233}xyz^2 + 4H_{1333}xz^3 + H_{2222}y^4$$

$$+4H_{2223}y^3z + 6H_{2233}y^2z^2 + 4H_{2333}yz^3 + H_{3333}z^4 \tag{6.6}$$

and

$$\begin{aligned}
p^{(8)}(t) = {} & (H_{1111} - 6H_{1122} + H_{2222} + 4i(-H_{1112} + H_{1222}))t^8 + \\
& 8(H_{1113} - 3H_{1223} + i(-3H_{1123} + H_{2223}))t^7 + \\
& 4(-H_{1111} + 6H_{1133} + H_{2222} - 6H_{2233} + 2i(H_{1112} + H_{1222} - 6H_{1233}))t^6 + \\
& 8(-3H_{1113} - 3H_{1223} + 4H_{1333} + i(3H_{1123} + 3H_{2223} - 4H_{2333}))t^5 + \\
& 2(3H_{1111} + 6H_{1122} - 24H_{1133} + 3H_{2222} - 24H_{2233} + 8H_{3333})t^4 + \\
& 8(3H_{1113} + 3H_{1223} - 4H_{1333} + i(3H_{1123} + 3H_{2223} - 4H_{3332}))t^3 + \\
& 4(-H_{1111} + 6H_{1133} + H_{2222} - 6H_{2233} + 2i(-H_{1112} - H_{1222} + 6H_{1233}))t^2 + \\
& 8(-H_{1113} + 3H_{1223} + i(-3H_{1123} + H_{2223}))t + \\
& H_{1111} - 6H_{1122} + H_{2222} + 4i(H_{1112} - H_{1222})
\end{aligned} \tag{6.7}$$

(6.7) has the form

$$p^{(8)}(t) = a_8t^8 + a_7t^7 + a_6t^6 + a_5t^5 + a_4t^4 - a_5{}^*t^3 + a_6{}^*t^2 - a_7{}^*t + a_8{}^*, \tag{6.8}$$

where $*$ denotes complex conjugate.

The coefficients in the 8th degree polynomial (6.7) in terms of elastic constants are given as:

$$\begin{aligned}
a_8 &= c_{11} + c_{22} - 4c_{66} - 2c_{12} + 4i(-c_{16} + c_{26}), \\
a_7 &= 8[c_{15} - c_{25} - 2c_{46} + i(-c_{14} + c_{24} - 2c_{56} - 3c_{23})], \\
a_6 &= 4[-c_{11} + c_{22} - 4c_{44} + 4c_{55} + 2c_{13} - 2c_{23} + 2i(c_{16} + c_{26} - 2c_{36} - 4c_{45})], \\
a_5 &= 8[-3c_{15} - c_{25} + 4c_{35} - 2c_{46} + i(c_{14} + 3c_{24} - 4c_{34} + 2c_{56}), \\
a_4 &= 2[3c_{11} + 3c_{22} + 8c_{33} - 16c_{44} - 16c_{55} + 4c_{66} + 2c_{12} - 8c_{13} - 8c_{23}], \\
a_3 &= -a_5^*, \qquad a_2 = a_6^*, \qquad a_1 = -a_7^*, \qquad a_0 = a_8^*.
\end{aligned} \tag{6.9}$$

The roots of the polynomials directly gives the space directions in the bouquet of vectors in Maxwell multipole. In Ch. 4 the magnitude is developed.

6.2.2 The 2nd rank harmonic tensors H_{ij} and h_{ij}

From Ch. 4, the fourth degree polynomial corresponding to H_{ij} and h_{ij} has the form

$$p^{(4)}(t) = a_4 t^4 + a_3 t^3 + a_2 t^2 - a_3^* t + a_4^*. \tag{6.10}$$

The coefficients a_i above related to H_{ij} are given as

$$\begin{aligned} a_4^{(H)} &= \frac{1}{21}[3c_{11} - 3c_{22} - 2c_{44} + 2c_{55} + c_{13} - c_{23} - 2i(3c_{16} + 3c_{26} + c_{36} + 2c_{45})], \\ a_3^{(H)} &= \frac{4}{21}[3c_{15} + c_{25} + 3c_{35} + 2c_{46} - i(c_{14} + 3c_{24} + 3c_{34} + 2c_{56})], \\ a_2^{(H)} &= \frac{2}{21}[-3c_{11} - 3c_{22} + 6c_{33} + 2c_{44} + 2c_{55} - 4c_{66} - 2c_{12} + c_{13} + c_{23}], \end{aligned} \tag{6.11}$$

which is the coefficients in the fourth degree polynomial associated with the totally symmetric part of the hierarchically symmetric tensor.

Further, the coefficients in the fourth degree polynomial associated with the non-totally symmetric part of the hierarchically symmetric tensor, h_{ij}, is given by

$$\begin{aligned} a_4^{(h)} &= \frac{2}{3}[c_{44} - c_{55} + c_{13} - c_{23} - 2i(c_{36} - c_{45})], \\ a_3^{(h)} &= \frac{16}{9}[c_{25} - c_{46} - i(c_{14} - c_{56})], \\ a_2^{(h)} &= \frac{4}{9}[c_{44} - 5c_{55} + 4c_{66} - 4c_{12} + 5c_{13} - c_{23}]. \end{aligned} \tag{6.12}$$

6.3 Perturbation of Maxwell multipoles

6.3.1 Norm of a tensor

For a given tensor, several derived quantities can be defined. One of the most familiar is the trace of a tensor with respect to a pair of indices. The problems dealing with here, is related to the definition of deviation of a derived quantity as a result of changing the tensor coefficients. In the following the change in vectors defined by Maxwell multipoles by a perturbation of a given tensor is analyzed. This gives a demonstration of the sensitivity of the multipoles gainst small changes in the tensor under consideration. Deviation from ideal symmetry in real data, causes deviation in the harmonic representation compared to ideal symmetry. A key-question here is how a perturbation of a given tensor can be done. This will be described in the following.

Norm-preserving mapping

The norm of two tensors T_{ijkl} and U_{ijkl} (inner product) is defined as $T_{ijkl}U_{ijkl}$, and the magnitude of a tensor T_{ijkl} is here defined as $\sqrt{T_{ijkl}T_{ijkl}}$.

The norm of a hierarchically symmetric tensor can be calculated by applying the norm-preserving mapping presented by Helbig (1996). Another reference for norm-preserving mapping is Mehrabadi and Cowin (1990). The hierarchically symmetric tensor can be mapped to a 21 dimensional vector, where the norm is preserved, in the following way:

$$C_A = \begin{pmatrix} C_I \\ C_{II} \\ C_{III} \\ C_{IV} \\ C_V \\ C_{VI} \\ C_{VII} \\ C_{VIII} \\ C_{IX} \\ C_X \\ C_{XI} \\ C_{XII} \\ C_{XIII} \\ C_{XIV} \\ C_{XV} \\ C_{XVI} \\ C_{XVII} \\ C_{XVIII} \\ C_{XIX} \\ C_{XX} \\ C_{XXI} \end{pmatrix} = \begin{pmatrix} c_{11} \\ c_{22} \\ c_{33} \\ \sqrt{2}c_{23} \\ \sqrt{2}c_{13} \\ \sqrt{2}c_{12} \\ 2c_{44} \\ 2c_{55} \\ 2c_{66} \\ 2c_{14} \\ 2c_{25} \\ 2c_{36} \\ 2c_{34} \\ 2c_{15} \\ 2c_{26} \\ 2c_{24} \\ 2c_{35} \\ 2c_{16} \\ 2\sqrt{2}c_{56} \\ 2\sqrt{2}c_{46} \\ 2\sqrt{2}c_{45} \end{pmatrix} \tag{6.13}$$

where c_{ij} are the familiar two-index Voigt notation of the hierarchically symmetric tensor. The factors in front of the coefficients c_{ij} reflect the number of identical coefficients in the hierarchically symmetric tensor. The square of each factor is equal to the number of coefficients identical in the four-index representation c_{ijkl}.

A hierarchically symmetric tensor is isomorphic to a 21 -dimensional vector. A perturbation of the tensor is in the following done by a 42 -step operation by adding to the vector a positive and a negative perturbation vector of equal magnitude in each of the 21 base directions in the 21- dimensional space. The magnitude is a fraction of the magnitude of the unperturbed vector under consideration. This approximates the overall distribution of errors: the endpoints of the perturbed vectors are evenly distributed on the 21-dimensional hyper sphere on the faces of the circumscribed hypercube (the corners of the inscribed hyper polyhedron (analog to 3D).

The matrix notation for the first four perturbation vectors with magnitude δ in symmetric matrix notation, $p^{(i)}$, are:

$$p^{(1)}_{\alpha\beta} = \begin{pmatrix} \delta & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \tag{6.14}$$

$$p^{(2)}_{\alpha\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ & \delta & 0 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \tag{6.15}$$

$$p^{(3)}_{\alpha\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 0 & 0 \\ & & \delta & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \tag{6.16}$$

$$p^{(4)}_{\alpha\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & \delta/\sqrt{2} & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \tag{6.17}$$

according to Voigt representation of a tensor in matrix form. In the same way e.g. $p^{(7)}$ is given as:

$$p^{(7)}_{\alpha\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & \delta/2 & 0 & 0 \\ & & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \tag{6.18}$$

In a similar way we get all the $p^{(i)}$ from $i = 1$ to 21.
For the next 21 $p^{(i)}$ we have

$$p^{(i+21)} = -p^{(i)}, \tag{6.19}$$

If the perturbation has magnitude δ, the 42 perturbations could be displayed as

$$P(\delta) = \begin{pmatrix} \delta & \delta/\sqrt{2} & \delta/\sqrt{2} & \delta/2 & \delta/2 & \delta/2 \\ & \delta & \delta/\sqrt{2} & \delta/2 & \delta/2 & \delta/2 \\ & & \delta & \delta/2 & \delta/2 & \delta/2 \\ & & & \delta/2 & \delta/2\sqrt{2} & \delta/2\sqrt{2} \\ & & & & \delta/2 & \delta/2\sqrt{2} \\ & & & & & \delta/2 \end{pmatrix} \tag{6.20}$$

where δ stands for a specific value and its value of opposite sign. Each of the 42 perturbations is performed when only one component is different from zero.

If the perturbation has unit magnitude, perturbation of component number IV, for instance, is the following:

$$C'_A = \begin{pmatrix} c_{11} \\ c_{22} \\ c_{33} \\ \sqrt{2}c_{23} \\ \sqrt{2}c_{13} \\ \sqrt{2}c_{12} \\ 2c_{44} \\ 2c_{55} \\ 2c_{66} \\ 2c_{14} \\ 2c_{25} \\ 2c_{36} \\ 2c_{34} \\ 2c_{15} \\ 2c_{26} \\ 2c_{24} \\ 2c_{35} \\ 2c_{16} \\ 2\sqrt{2}c_{56} \\ 2\sqrt{2}c_{46} \\ 2\sqrt{2}c_{45} \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{6.21}$$

Thus

$$C'_{IV} = \sqrt{2}c_{23} + 1$$

Mapped to the matrix notation, the perturbed c_{23}, c'_{23}, is

$$c'_{23} = C'_{IV}/\sqrt{2} = (\sqrt{2}c_{23} + 1)/\sqrt{2} = c_{23} + 1/\sqrt{2}.$$

6.4 Analysis of perturbation

The harmonic decomposition consists of one fourth rank tensor, $H^{(4)}$, two 2nd rank tensors, $H^{(2)}$ and $h^{(2)}$ and two scalars. Maxwell multipole for $H^{(4)}$ is characterized by a bouquet of four 3-dimensional vectors. Correspondingly, each of $H^{(2)}$ and $h^{(2)}$ are characterized with a bouquet of two vectors.

6.4.1 Triclinic symmetry

The following tensor of triclinic symmetry (tricl.q) is analyzed:

$$c^{tricl} = \begin{pmatrix} 3.150 & 1.950 & 1.850 & 2.000 & 2.000 & 1.100 \\ & 2.750 & -1.350 & 1.100 & 1.200 & 1.000 \\ & & 6.650 & 1.000 & 1.300 & 2.000 \\ & & & 2.550 & 1.000 & 1.000 \\ & & & & 2.600 & 1.350 \\ & & & & & 2.450 \end{pmatrix} \tag{6.22}$$

To check whether the tensor has higher symmetry than monoclinic, rotation to a coordinate system with eigenvectors of one 2nd rank tensor derived from c^{tricl} is done. The tensor still has 21 coefficients. See Cp. 2 for further discussion. The magnitude of the tensor is 16.298.

<u>5 % perturbation.</u>
5 % of the magnitude is 0.8149. Each of the tensors representing the perturbation have the norm 0.8149, and in matrix representation each component is zero except one of them and given according to (6.20).

In the following perturbation is performed according to the process described in section 6.3. As an example, two of the 42 perturbations then become:

$$c_{p1}^{tricl} = c^{tricl} + p^{(1)} =$$

$$\begin{pmatrix} 3.965 & 1.950 & 1.850 & 2.000 & 2.000 & 1.100 \\ & 2.750 & -1.350 & 1.100 & 1.200 & 1.000 \\ & & 6.650 & 1.000 & 1.300 & 2.000 \\ & & & 2.550 & 1.000 & 1.000 \\ & & & & 2.600 & 1.350 \\ & & & & & 2.450 \end{pmatrix} \tag{6.23}$$

$$c_{p4}^{tricl} = c^{tricl} + p^{(4)} =$$

$$\begin{pmatrix} 3.150 & 1.950 & 1.850 & 2.000 & 2.000 & 1.100 \\ & 2.750 & -0.7738 & 1.100 & 1.200 & 1.000 \\ & & 6.650 & 1.000 & 1.300 & 2.000 \\ & & & 2.550 & 1.000 & 1.000 \\ & & & & 2.600 & 1.350 \\ & & & & & 2.450 \end{pmatrix} \tag{6.24}$$

Matrix	Magnitude		Relative Dev. in %		Angular Dev. in deg.	
position	Pos.pert.	Neg.pert.	Pos. pert.	Neg. pert.	Pos. pert.	Neg. pert.
11	21.918	22.970	2.9	3.1	1.1	1.0
22	22.246	22.600	5.9	6.0	3.4	3.4
33	22.789	22.046	2.1	2.1	0.7	0.9
23	21.921	22.934	4.6	4.3	2.4	2.1
13	22.441	22.466	2.1	1.9	1.2	1.2
12	23.172	21.657	5.5	5.9	2.4	2.9
44	21.739	23.161	6.6	6.1	3.4	2.9
55	22.485	22.516	3.0	3.0	1.7	1.7
66	23.493	21.354	7.8	8.5	3.4	4.2
14	23.058	21.868	5.4	4.9	2.6	2.5
25	22.606	22.294	6.1	5.9	3.5	3.4
36	23.649	21.192	6.8	6.8	2.2	2.5
34	21.790	23.315	4.8	5.4	2.3	2.0
15	23.274	21.549	5.0	5.1	1.8	2.1
26	21.993	23.079	8.7	9.4	4.9	5.0
24	22.690	22.360	7.5	8.6	4.2	5.0
35	21.451	23.153	5.1	3.8	1.6	0.4
16	21.845	23.205	5.6	5.8	3.1	2.6
56	23.367	21.673	7.7	6.9	3.7	3.5
46	22.717	22.271	8.6	8.4	4.8	4.8
45	24.172	20.697	9.6	9.7	3.0	3.6

Table 6.1: $H^{(4)}$. Magnitude, relative deviation in % , and angular deviation relative to the unperturbed vector for each of the 42 perturbations.

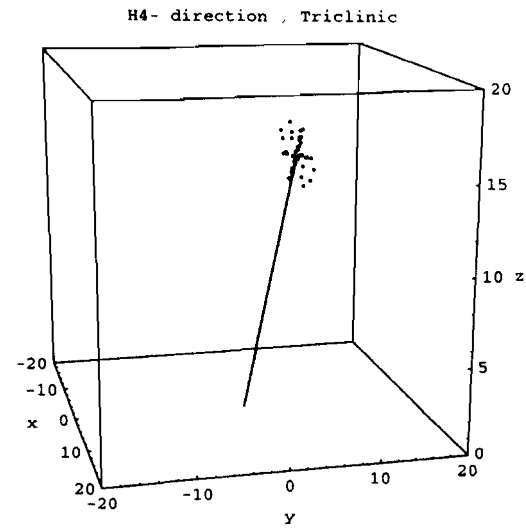
$\underline{H^{(4)}}$.

Fig. 6.1 shows the perturbation of one of the vectors in the $H^{(4)}$ -bouquet, together with the unperturbed vector. The dots are the endpoints of the perturbed vector, and the solid line is the unperturbed vector. Fig. 6.2 shows a "zoomed" version of Fig. 6.1 with two different viewpoints. The figure shows that the 42 perturbations are not equal. The perturbations vary in angle and magnitude.

The magnitude of the difference between the vectors relative to the the magnitude of the vector in the unperturbed state (relative deviation in %) is calculated. The result is presented in Table 6.1.

Angular deviation of the direction in the multipole relative to the direction in the unperturbed state is shown as well. The chosen $H^{(4)}-$ vector is: $[15.060, 1.884, 16.482]$, such that the magnitude is 22.406.

The maximum, minimum and average relative deviation is, respectively, 9.7 % , 1.9 % and 5.8 % . Maximum and minimum values occur respectively for c_{45} and c_{13}.



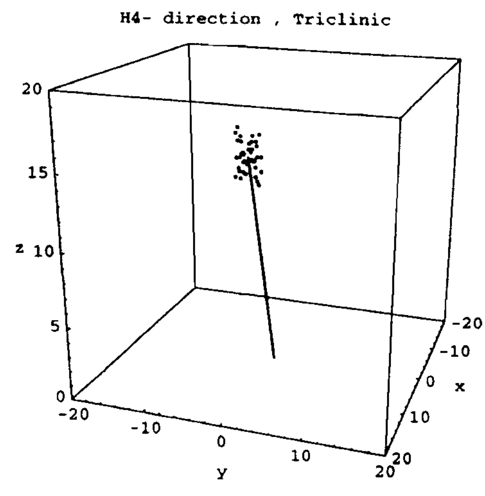


Figure 6.1: Perturbation of one $H^{(4)}$ -vector with two different viewpoints.

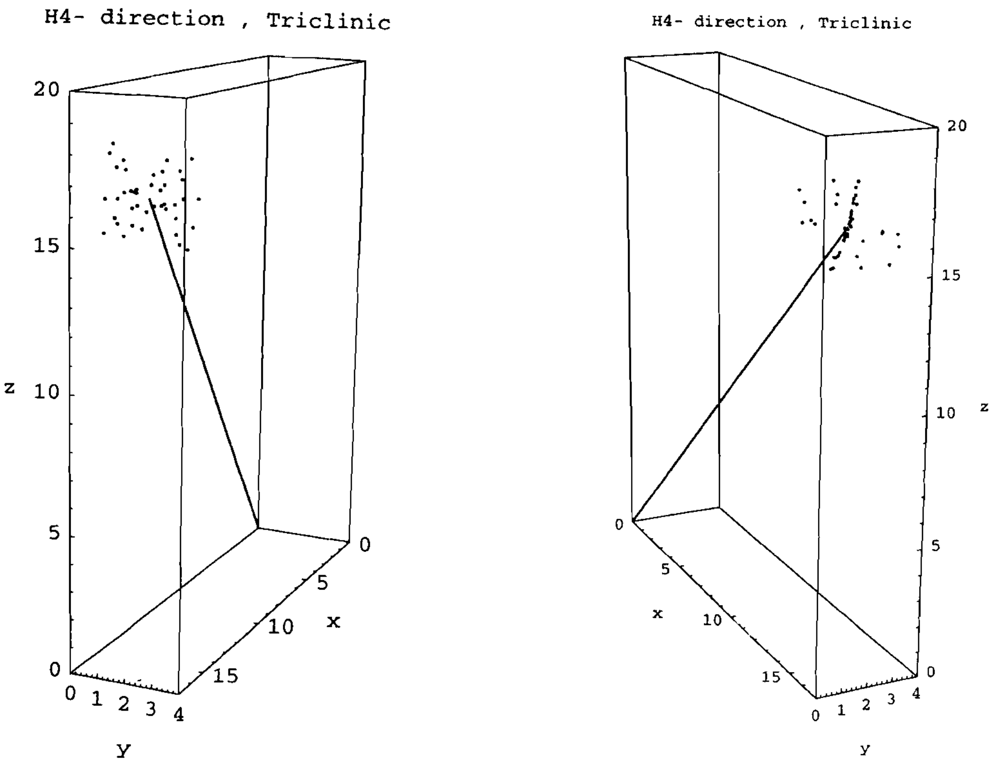


Figure 6.2: "Zoomed" versions of Fig. 6.1.

Matrix position	Magnitude Pos.pert.	Magnitude Neg.pert.	Relative Dev. in % Pos. pert.	Relative Dev. in % Neg. pert.	Angular Dev in deg. Pos. pert.	Angular Dev in deg. Neg. pert.
11	1.8049	1.8153	5.6	5.1	3.3	3.2
22	1.7596	1.8577	11.3	10.6	6.5	6.1
33	1.8570	1.7445	6.4	7.2	3.2	3.8
23	1.8003	1.7980	1.3	1.3	0.8	1.3
13	1.8111	1.7870	2.6	2.6	1.8	1.6
12	1.7853	1.8119	1.6	1.6	0.9	1.1
44	1.8015	1.7982	2.2	1.9	0.6	0.5
55	1.8166	1.7825	3.6	3.7	2.0	2.3
66	1.7800	1.8175	2.3	2.2	0.6	1.5
14	1.8135	1.7853	2.7	2.8	1.7	1.5
25	1.8127	1.7852	2.1	2.0	1.8	0.9
36	1.8269	1.7705	2.9	3.1	1.8	1.4
34	1.8496	1.7635	8.4	7.9	4.2	4.7
15	1.8446	1.7604	6.6	5.6	3.4	3.4
26	1.8845	1.7168	8.4	10.1	4.6	5.3
24	1.8496	1.7635	8.5	8.1	4.3	4.7
35	1.8446	1.7710	6.7	4.1	3.5	2.5
16	1.8845	1.7168	8.4	10.1	4.0	5.3
56	1.8203	1.7804	3.9	3.7	2.0	1.7
46	1.8189	1.7798	3.1	2.8	1.8	1.7
45	1.8388	1.7591	4.1	4.5	2.3	2.6

Table 6.2: $H^{(2)}$. Magnitude, relative deviation in % , and angular deviation relative to the unperturbed vector for each of the 42 perturbations.

Magnitude as well as direction of the multipole are perturbed. The angular deviation is within 5 % .

$\underline{H^{(2)}}$.

Table 6.2 shows magnitude, relativ deviation and angular deviation for one of the vectors in the multipole bouquet for $H^{(2)}$. For the unperturbed tensor, the chosen multipole vector is [1.274, 0.3323, 1.225] with magnitude 1.7985.

The maximum, minimum and average relative deviation is, respectively, 11.3 % , 1.3 % and 4.9 % . Maximum and minimum values occur respectively for c_{22} and c_{23}.

$\underline{h^{(2)}}$.

Table 3 is the corresponding table for $h^{(2)}$. For the unperturbed tensor, the chosen multipole vector is [2.5677, −0.30292, 1.2910] with magnitude 2.8892.
The maximum, minimum and average relative deviation is, respectively, 21.0 % , 0

Matrix	Magnitude		Relative Dev. in %		Angular Dev. in deg.	
position	Pos.pert.	Neg.pert.	Pos. pert.	Neg. pert.	Pos. pert.	Neg. pert.
11	2.8892	2.8892	0	0	0	0
22	2.8892	2.8892	0	0	0	0
33	2.8892	2.8892	0	0	0	0
23	2.5573	3.2351	12.0	12.4	2.3	1.3
13	3.0878	2.7818	16.2	15.4	8.2	8.6
12	3.1214	2.7493	14.1	13.1	6.4	7.3
44	3.1327	2.6527	8.7	8.5	1.5	1.7
55	2.8040	3.0210	11.0	11.4	6.1	5.9
66	2.7814	3.0444	9.4	9.9	5.1	4.7
14	3.1756	2.6102	19.8	21.0	9.4	11.2
25	2.9276	2.9290	9.6	8.4	5.4	4.7
36	3.1298	2.7245	12.5	11.7	5.0	5.9
34	2.8892	2.8892	0	0	0	0
15	2.8892	2.8892	0	0	0	0
26	2.8892	2.8892	0	0	0	0
24	2.8892	2.8892	0	0	0	0
35	2.8892	2.8892	0	0	0	0
16	2.8892	2.8892	0	0	0	0
56	2.6912	3.0909	16.7	14.3	9.1	6.9
46	2.9091	2.9083	6.0	6.6	3.2	3.7
45	2.7645	3.0518	8.3	8.7	4.1	3.7

Table 6.3: $h^{(2)}$. Magnitude, relative deviation in % , and angular deviation relative to the unperturbed vector for each of the 42 perturbations.

% and 6.8 % . Maximum value occur for c_{14}.

The table shows that there is no perturbation of the multipole $h^{(2)}$ for perturbation of the following components of the elastic tensor: c_{11}, c_{22}, c_{33}, c_{34}, c_{15}, c_{26}, c_{24}, c_{35} and c_{16}. Those components are completely determined by the totally symmetric part of the hierarchically symmetric tensor (as we shall see in the following). $h^{(2)}$ is related to the non-totally symmetric tensor, which is in accordance with Ch. 2, where the totally- and non-totally symmetric part of HST are represented respectively as

$$s_{ij} = \begin{pmatrix} c_{11} & s_{66} & s_{55} & s_{56} & c_{15} & c_{16} \\ & c_{22} & s_{44} & c_{24} & s_{46} & c_{26} \\ & & c_{33} & c_{34} & c_{35} & s_{45} \\ & & & s_{44} & s_{45} & s_{46} \\ & & & & s_{55} & s_{56} \\ & & & & & s_{66} \end{pmatrix}$$

and

$$a_{ij} = \begin{pmatrix} 0 & -2a_{66} & -2a_{55} & -2a_{56} & 0 & 0 \\ & 0 & -2a_{44} & 0 & -2a_{46} & 0 \\ & & 0 & 0 & 0 & -2a_{45} \\ & & & a_{44} & a_{45} & a_{46} \\ & & & & a_{55} & a_{56} \\ & & & & & a_{66} \end{pmatrix}$$

We notice that the nine terms s_{11}, s_{22}, s_{33}, s_{34}, s_{15}, s_{26}, s_{24}, s_{35}, and s_{16} are all equal to the corresponding elastic components, and the corresponding non-totally symmetric contributions are zero.

Eq. (6.12) also shows that the remaining 12 elastic components contribute to the polynomial determining the bouquet of space directions accociated to $h^{(2)}$.

The above discussion also highlights the following physical significance of the totally-/non-totally symmetric part of HST: The following elastic components are determined completely by the totally symmetric part of HST:

1. The three elastic components connecting compressional stress σ_{pp} (no summation over p), $p = 1, 2, 3$ with the compressional strain of the same kind, ϵ_{pp}.

2a. The six elastic components connecting compressional stress σ_{pp} and shear strain ϵ_{pq}, $q \neq p$.

2b. The six elastic components in 2a are also connecting compressional strain ϵ_{pp}, and shear stress σ_{pq}, $q \neq p$. This point is taken care of by the symmetry of HST.

The remaining 12 (independent) elastic components are determined by the totally symmetric part as well as of the non-totally symmetric part of HST.

In four-subscript notation the nine elastic components above, determined by the totally symmetric part, is C_{1111}, C_{2222}, C_{3333}, C_{3323}, C_{1113}, C_{2212}, C_{2223}, C_{3313}, C_{1112}. For a HST tensor, each elastic component above are invariant against any permutation of its indices. Those nine elastic components are the only where any permutation of the four subscripts in each set gives the same elastic constant.

For permutations of the elastic constants determined by the totally- as well as the non-totally symmetric part, the deviations in the multipoles are much larger for $h^{(2)}$ than for $H^{(4)}$ and $H^{(2)}$. However , the average value of the relative deviation is close to the values for $H^{(4)}$ and $H^{(2)}$.

6.4.2 Orthorhombic symmetry

The following tensor of orthorhombic symmetry (ortho.q) is analyzed:

$$c^{ortho} = \begin{pmatrix} 3.150 & 1.950 & 1.850 & 0.000 & 0.000 & 0.000 \\ & 2.750 & -1.350 & 0.000 & 0.000 & 0.000 \\ & & 6.650 & 0.000 & 0.000 & 0.000 \\ & & & 2.550 & 0.000 & 0.000 \\ & & & & 2.600 & 0.000 \\ & & & & & 2.450 \end{pmatrix} \tag{6.25}$$

The symmetry axes are parallel to the coordinate axes. In the following the effect of perturbation of elastic constants on the symmetry elements determined by Maxwell multipoles is analysed. The analysis is numerical, rather than graphical. However, for orthorhombic symmetry, it is easy to imagine graphical representation related to the main content of the analysis specially if the coordinate system is in the symmetry coordinate system. Use of symmetry coordinate system is a matter of convenience. The internal structure of the vectors in the multipole bouquet is independent of coordinate system.

Generally the vectors in the bouquets of the multipoles occur as pairs symmetric about possible symmetry axes. For $H^{(4)}$, in addition to the four vectors, there are four vectors pointing in the opposite directions.

In the following analysis, a bouquet of four vectors are used. For each vector, there exists a vector such that the two vectors together occur symmetric about a symmetry axis. Summation of each unit vector with each of the other unit vectors in the bouquet would reveal symmetry dirctions for the orthorhombic tensor. With four vectors, there are six possible combinations of adding pairwise two vectors. See Table 6.4 for the bouquet of four vectors, and Table 6.5 for the sum-vectors in the unperturbed state. By inspection, one of the sum-vectors is parallel to the x -axis, and one is parallel to the z -axis. In the selection process of four vectors in the bouquet, combinations of two vectors could be replaced by the opposite directions. Still two of the sum-vectors are parallel to coordinate axes, although not nececcarily the x - and z -axes.

By applying at least one of the four opposite vectors in the bouquet, all three symmetry axes would be defined. In that case the number of combinations in the summation process would be high and more complicated to deal with in the analysis. In addition to the summation process, the angle between each of the sum-vectors will be calculated. In the unperturbed state, one of the angles are 90 degrees. The 15 angles between sum-vectors are shown in Table 6.6 (unperturbed state).

No.	Unit vectors in the $H^{(4)}$ – bouquet
1	[0.84469, 0, 0.53525]
2	[0.62717, 0.77888, 0]
3	[0.62717, −0.77888, 0]
4	[−0.84469, 0, 0.53525]

Table 6.4: Bouquet of four vectors in the multipole, orthorhombic symmetry (ortho.q), unperturbed state.

No.	Sum – vectors ($H^{(4)}$)
1	[1.4719, 0.77888, 0.53525]
2	[1.4719, −0.77888, 0.53525]
3	[0, 0, 1.0705]
4	[1.2543, 0, 0]
5	[−0.21752, 0.77888, 0.53525]
6	[−0.21752, −0.77888, 0.53525]

Table 6.5: Sum-vectors for the four vectors in Table 6.4.

52.88	72.18	32.70	70.26	112.18
72.18	32.70	112.18	70.26	90.00
56.50	56.50	102.96	102.96	106.86

Table 6.6: Mutual angles between the six sum-vectors for ortho.q.

No.	Unit vectors in the $H^{(4)}$ – bouquet
1	[0.84064, 0, 0.54159]
2	[0.60158, −0.79881, 0]
3	[0.60158, 0.79881, 0]
4	[−0.84064, 0, 0.54159]

Table 6.7: Bouquet of four vectors in the multipole, perturbed state.

No.	Sum – vectors ($H^{(4)}$)
1	[1.4422, −0.79881, 0.54159]
2	[1.4422, 0.79881, 0.54159]
3	[0, 0, 1.0832]
4	[1.2032, 0, 0]
5	[−0.23906, −0.79881, 0.54159]
6	[−0.23906, 0.79881, 0.54159]

Table 6.8: Sum-vectors for the four vectors, perturbed state.

Only one angle is 90 degrees, and we will pay special attention to this angle under the perturbation process. Also the two sum-vectors parallel to coordinate axes respectively are analysed in the following.

5 % perturbation.

The norm of the tensor is 12.5244. 5 % of the norm is 0.62622. Similar to the 42-step perturbation process for triclinic symmetry, perturbation is performed for orthorhombic symmetry. What is analysed however in this case, is how symmetry elements are perturbed by perturbation of elastic constants. By a perturbation of c_{11} by 0.62622, similar tables to the tables 4, 5 and 6 are:

All directions and angles are changed except sum-vectors parallel to the $x-$ and $z-$ axes, and accordingly the angle between them. Obviously the directions of symmetry axes are not changed by changing c_{11}. But what happens when vanishing

54.82	71.81	33.79	70.12	113.56
71.81	33.79	113.56	70.12	90.00
56.99	56.99	103.91	103.91	106.91

Table 6.9: Mutual angles between the six sum-vectors, perturbed state.

Matrix position	$\Delta \mathbf{v}_1$in deg. Pos.pert.	Neg.pert.	$\Delta \mathbf{v}_2$in deg. Pos. pert.	Neg. pert.	$\Delta\alpha$ in deg. Pos. pert.	Neg. pert.
11	0	0	0	0	0	0
22	0	0	0	0	0	0
33	0	0	0	0	0	0
23	0	0	0	0	0	0
13	0	0	0	0	0	0
12	0	0	0	0	0	0
44	0	0	0	0	0	0
55	0	0	0	0	0	0
66	0	0	0	0	0	0
14	4.6	4.6	0	0	0	0
25	4.5	4.5	0	4.5	0	9.0
36	4.6	4.6	0	0	0	0
34	10.7	9.7	0	0	0	0
15	6.8	6.8	1.3	1.3	5.5	5.5
26	1.8	1.8	0	0	0	0
24	13.9	13.9	0	0	0	0
35	3.2	3.2	11.4	0	14.6	0
16	2.8	2.8	0	0	0	0
56	6.5	6.5	0	0	0	0
46	6.3	6.3	0	6.3	0	12.6
45	6.6	6.6	0	0	0	0

Table 6.10: Deviation from symmetry axes for two sum-vectors. Deviation from 90 degrees between the two sum-vectors are shownn as well. The sign of the deviation is not taken into account.

elastic components change? In the following the remaining 41 perturbations are performed, and the effect on the original symmetry axes and the angle between them are shown.

By using a bouquet of four vectors, two symmetry axes are defined by the summation process. In table 6.10 the deviation from each of the symmetry axes (which in this case are parallel to coordinate axes) are shown. We call the two symmetry axes $\mathbf{v}_1$ and $\mathbf{v}_2$. In addition the deviation from 90 degrees are shown.

Appendix

LIST OF SPHERICAL HARMONICS.

Harmonic tensors are related to Solid Spherical Harmonics. A Solid Spherical Harmonic is a homogeneous function of degree n satisfying the Laplace's differential equation

$$\nabla^2 V = 0 \tag{A-1}$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. A function $f(x, y, z)$ is homogeneous of degree n if $f(\lambda x, \lambda y, \lambda z) = \lambda^n f(x, y, z)$. This is a formal definition of a homogeneous function where n has any value real or complex.
The ordinary Solid Spherical Harmonics are polynomials of positive integer degree.
In the following a list of Surface Spherical Harmonics up to order four is given. The list is based on the development in Kovach (1982), Hobson (1955) and Sagan (1961). The factors due to normalizing on the sphere is not included.

$$Y_0^0(\theta, \phi) = 1 \tag{A-2}$$

$$Y_1^0(\theta, \phi) = \cos\theta \tag{A-3}$$

$$Y_1^{1c}(\theta, \phi) = \sin\theta\cos\phi \tag{A-4}$$

$$Y_1^{1s}(\theta, \phi) = \sin\theta\sin\phi \tag{A-5}$$

$$Y_2^0(\theta, \phi) = \frac{1}{2}(3\cos^2\theta - 1) \tag{A-6}$$

$$Y_2^{1c}(\theta, \phi) = 3\cos\theta\sin\theta\cos\phi \tag{A-7}$$

$$Y_2^{1s}(\theta, \phi) = 3\cos\theta\sin\theta\sin\phi \tag{A-8}$$

$$Y_2^{2c}(\theta, \phi) = 3\sin^2\theta\cos 2\phi \tag{A-9}$$

$$Y_2^{2s}(\theta, \phi) = 3\sin^2\theta\sin 2\phi \tag{A-10}$$

$$Y_3^0(\theta,\phi) = \frac{1}{2}(5\cos^3\theta - 3\cos\theta) \tag{A-11}$$

$$Y_3^{1c}(\theta,\phi) = \frac{3}{2}\sin\theta(5\cos^2\theta - 1)\cos\phi \tag{A-12}$$

$$Y_3^{1s}(\theta,\phi) = \frac{3}{2}\sin\theta(5\cos^2\theta - 1)\sin\phi \tag{A-13}$$

$$Y_3^{2c}(\theta,\phi) = 15\cos\theta\sin^2\theta\cos 2\phi \tag{A-14}$$

$$Y_3^{2s}(\theta,\phi) = 15\cos\theta\sin^2\theta\sin 2\phi \tag{A-15}$$

$$Y_3^{3c}(\theta,\phi) = 15\sin^3\theta\cos 3\phi \tag{A-16}$$

$$Y_3^{3s}(\theta,\phi) = 15\sin^3\theta\sin 3\phi \tag{A-17}$$

$$Y_4^0(\theta,\phi) = \frac{1}{8}(35\cos^4\theta - 30\cos^2\theta + 3) \tag{A-18}$$

$$Y_4^{1c}(\theta,\phi) = \frac{5}{2}\sin\theta(7\cos^3\theta - 3\cos\theta)\cos\phi \tag{A-19}$$

$$Y_4^{1s}(\theta,\phi) = \frac{5}{2}\sin\theta(7\cos^3\theta - 3\cos\theta)\sin\phi \tag{A-20}$$

$$Y_4^{2c}(\theta,\phi) = 15\sin^2\theta(7\cos^2\theta - 1)\cos 2\phi \tag{A-21}$$

$$Y_4^{2s}(\theta,\phi) = 15\sin^2\theta(7\cos^2\theta - 1)\sin 2\phi\sin 2\phi \tag{A-22}$$

$$Y_4^{3c}(\theta,\phi) = \frac{105}{2}\sin^3\theta\cos\theta\cos 3\phi \tag{A-23}$$

$$Y_4^{3s}(\theta,\phi) = \frac{105}{2}\sin^3\theta\cos\theta\sin 3\phi \tag{A-24}$$

$$Y_4^{4c}(\theta,\phi) = \frac{105}{2}\sin^4\theta\cos 4\phi \tag{A-25}$$

$$Y_4^{4s}(\theta,\phi) = \frac{105}{2}\sin^4\theta\sin 4\phi \tag{A-26}$$

A list of solid spherical harmonics in Cartesian coordinates up to degree 4 is given as follows:

$$\Psi_0^0(x,y,z) = 1 \tag{A-27}$$

$$\Psi_1^0(x,y,z) = z \tag{A-28}$$

$$\Psi_1^{1c}(x,y,z) = x \tag{A-29}$$

$$\Psi_1^{1s}(x,y,z) = y \tag{A-30}$$

$$\Psi_2^0(x,y,z) = z^2 - \frac{1}{2}(x^2+y^2) \tag{A-31}$$

$$\Psi_2^{1c}(x,y,z) = xz \tag{A-32}$$

$$\Psi_2^{1s}(x,y,z) = yz \tag{A-33}$$

$$\Psi_2^{2c}(x,y,z) = x^2 - y^2 \tag{A-34}$$

$$\Psi_2^{2s}(x,y,z) = xy \tag{A-35}$$

$$\Psi_3^{0}(x,y,z) = -3x^2z - 3y^2z + 2z^3 \tag{A-36}$$

$$\Psi_3^{1c}(x,y,z) = -x^3 - xy^2 + 4xz^2 \tag{A-37}$$

$$\Psi_3^{1s}(x,y,z) = -x^2y - y^3 + 4yz^2 \tag{A-38}$$

$$\Psi_3^{2c}(x,y,z) = -x^2z - y^2z \tag{A-39}$$

$$\Psi_3^{2s}(x,y,z) = xyz \tag{A-40}$$

$$\Psi_3^{3c}(x,y,z) = x^3 - 3xy^2 \tag{A-41}$$

$$\Psi_3^{3s}(x,y,z) = 3x^2y - y^3 \tag{A-42}$$

$$\Psi_4^{0}(x,y,z) = 3x^4 + 6x^2y^2 - 24x^2z^2 + 3y^4 - 24y^2z^2 + 8z^4 \tag{A-43}$$

$$\Psi_4^{1rmc}(x,y,z) = 3x^3z + 3xy^2z - 4xz^3 \tag{A-44}$$

$$\Psi_4^{1s}(x,y,z) = 3x^2yz + 3y^3z - 4yz^3 \tag{A-45}$$

$$\Psi_4^{2c}(x,y,z) = x^4 - 6x^2z^2 - y^4 + 6y^2z^2 \tag{A-46}$$

$$\Psi_4^{2s}(x,y,z) = x^3y + xy^3 - 6xyz^2 \tag{A-47}$$

$$\Psi_4^{3c}(x,y,z) = x^3z - 3xy^2z \tag{A-48}$$

$$\Psi_4^{3s}(x,y,z) = y^3z - 3x^2yz \tag{A-49}$$

$$\Psi_4^{4c}(x,y,z) = x^4 - 6x^2y^2 + y^4 \tag{A-50}$$

$$\Psi_4^{4s}(x,y,z) = x^3y - xy^3 \tag{A-51}$$

Conclusion

The topic of my thesis has been coordinate-free representation of the anisotropic elastic tensor in order to describe and determine symmetry properties of the corresponding medium. A contribution to better understand fundamentals which could represent tools in solving problems in the determination of symmetry properties from the elastic tensor itself has been intended.

The elastic tensor is a fourth rank tensor in three dimensions, with the symmetry properties given by $E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}$. To describe real media, it has to satisfy stability conditions as well.

In the multipole formalism – described below and throughout the thesis – stability conditions of the fourth rank tensor in three dimension is not taken into account. A fourth rank tensor in three dimensions satisfying the symmetry conditions for elastic tensors is here defined as a hierarchically symmetric tensor (HST). In this definition stability conditions need not be satisfied. In the following, stability conditions are not taken into account, so we are talking about a HST.

My work on coordinate-free representation is mainly based on Backus (1970) including Maxwell multipoles. The theory is based on a specified decomposition of the HST tensor into harmonic tensors, and Maxwell multipoles are the geometrical representation of the harmonic tensor in 3-dimensional space. This representation consists of bouquets of 3-dimensional vectors in addition to two scalars. This thesis contains applications and further developments of his theory.

The internal structure of the bouquets of 3-dimensional vectors is independent of the coordinate system the tensor is referred to. Thus the directions defined by the vectors and the magnitude are independent of the orientation of the coordinate system. Those properties are said to be coordinate-free. Another example of coordinate-free property is the structure of eigenvectors of 2nd rank tensors associated to the HST (see Ch. 5).

An important concept in the multipole formalism is total symmetry. In a totally symmetric fourth rank tensor, T_{ijkl}, all tensor components with specific indices i, j, k and l are equal regardless the permutation of the indices. A comparison of different decompositions of the HST tensor has been done, and published. After a discussion on totally symmetry, a Corrigendum was puplished by Cowin (1993).

This thesis contains a review of the multipole concept developed by Maxwell (1881), the connection to the spherical harmonics and how they can be used in the tensor analysis of elastic tensors. In the tensor analysis concepts from modern algebra is applied. Modern algebra, like group theory, seems to be important in further development of the theory of elastic anisotropy.

In Ch. 4 a classification of symmetry classes by means of the structure of the vectors in the bouquets is given, and the magnitude of the bouquets of 3-dimensional vectors are derived.

Examples have been given where multipoles are displayed, and the coordinate free property of the multipoles is shown. The magnitude of the bouquets of 3-dimensional vectors are derived. The formulas giving the magnitude has been implemented in the software as well, and applied in Ch 6, where perturbation is discussed.

Since the magnitude of the vectors vanish for isotropic symmetry, further development might include magnitude as a measure for deviation from isotropy. Only the two scalars in the harmonic decomposition determine the two independent components of a tensor of isotropic symmetry.

Several 2nd rank tensors related to the elastic tensor are investigated with respect to eigenvectors, and a classification of eigenvectors for different symmetries are given in Ch. 5. For monoclinic and higher symmetry, there exist always eigenvectors aligned with symmetry axes and normals to symmetry planes. The deviatoric parts of the 2nd rank tensors considered in th enalysis vanish for cubic and isotropic symmetry, and might become a tool in defining deviation from isotropic or cubic symmetry.

In the vectorspace of hierarchically symmetric fourth rank tensors, a basis of 21 orthonormal base tensors are defined in Ch. 3. The base tensors are derived from spherical harmonics. A decomposition of the elastic tensor into the 21 base tensors for different symmetry classes is presented.

Most of my work is related to ideal media, with symmetry properties as in crystal physics. In Ch. 6 modelling of measuring real data is performed by perturbation of tensors of ideal symmetry. Perturbation of a triclinic tensor models measuring inaccuracy.

Perturbation of ta HST tensor indicates if the multipoles are "stable". A perturbation of five percent for a specific tensor of triclinic symmetry effect the different multipoles to deviate approximately the same amount with the definition of deviation I have applied. The deviations are 5.8 % , 4.9 % and 6.8 % for one vector in the bouquet for $H^{(4)}, H^{(2)}$, and $h^{(2)}$ respectively. An example is also given for a tensor of orthorhombic symmetry, where it is shown how much symmetry elements change by perturbation of the tensor.

Perturbation of a tensor of ideal higher symmetry, models deviation from ideal symmetry. Further work has to be done in applying the fundamentals to obtain measures of deviation from ideal symmetry.

Parts of the work have been published as two papers, and a third paper has been accepted, and is in press.

Samenvatting (Summary in Dutch)

Algemene elasticiteit theorie moet noodzakelijkerwijs rekening houden met de richting-afhankelijkheid van de eigenschappen. Wanneer in een medium een bepaalde eigenschap afhangt van de richting, dan is dit medium anisotroop voor deze eigenschap. Voorbeelden van elastische media zijn gesteenten en materialen gebruikt in de constructie industrie en de biologische wetenschap.

Het begrip tensor vormt voor de elastische anisotropie het meest fundamentele begrip. Alhoewel een tensor een fysische eigenschap beschrijft en als zodanig onafhankelijk is van coordinaten stelsels, kan een tensor voorgesteld worden door componenten die gedefinieerd zijn ten opzichte van een coordinaten stelsel. Een vector - hetgeen een eerste orde tensor is - is de meest bekende grootheid waarvan de componenten afhangen van het coordinaten stelsel. Tezamen vormen de componenten de tensor. Een skalaire grootheid zoals de lengte van een vector, is onafhankelijk van het coordinaten stelsel ten opzichte waarvan de vector is gedefinieerd. De lengte van de vector is een coordinaat-onafhankelijke grootheid.

Het onderwerp van mijn proefschrift is de coordinaat-onafhankelijke representatie van de anisotrope elasticiteit tensor, met als doel de symmetrie eigenschappen van het betreffende medium te beschrijven en te bepalen. Het is gepoogd een bijdrage te leveren aan een beter begrip van de fundamentele principes, die gebruikt zouden kunnen worden voor de bepaling van de symmetrie eigenschappen van de elasticiteit tensor.

De elasticiteit tensor is een drie dimensionale tensor van de vierde orde, met symmetrie eigenschappen bepaald door $E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij}$. Om echte media te beschrijven moet het ook aan stabiliteit condities voldoen. In een willekeurig coordinaten stelsel heeft de elasticiteit tensor 21 elementen die niet nul zijn. De isotrope tensor vormt een uitzondering omdat sommige elementen nul zijn ongeacht het coordinaten stelsel en de tensor slechts twee onafhankelijke elementen bevat. Voor een ideaal medium met een bepaalde symmetrie bestaan er coordinaten stelsels waarbij sommige elementen nul zijn. Voor experimenteel bepaalde tensoren zijn er geen elementen die nul kunnen worden vanwege afwijkingen van de ideale symmetrie en onnauwkeurigheden in de metingen. Daarom zijn er voor realistische media 21 elementen in ieder willekeurig coordinaten stelsel.

Het is de vraag hoe voor een elastisch anisotroop materiaal de symmetrie bepaald kan worden uit de componenten van de elasticiteit tensor. Hoe kan een coordinaten stelsel gevonden worden waarbij het aantal constanten vermindert, en wat kan gezegd worden over de symmetrie? Deze vragen vormden de motivatie om algemene theorieen te bestuderen waarmee mogelijk deze en gerelateerde problemen opgelost zouden kunnen worden.

Een theorie om de elasticiteit tensor op een geometrische manier weer te geven werd gegeven door Backus (1970). De theorie is gebaseerd op een specifieke decompositie van de elasticiteit tensor in harmonische tensoren. Harmonische decompositie wordt ook op andere manieren gedaan, zoals bijvoorbeeld in Mochizuki (1988) en Cowin (1989) (zie hoofdstuk 2).

Kelvin (1856) en Sutcliffe (1992) beschrijven decomposities van de elasticiteit tensor door middel van eigentensoren en eigenstijfheden. Het principe werd voorgesteld door Kelvin (1856), maar schijnt destijds niet geaccepteerd te zijn. Het werd onafhankelijk ontdekt door Pipkin (1976), Rychlewsky (1984), Mehrabadi en Cowin (1990) en Sutcliffe (1992). Een grondige discussie wordt gegeven in Helbig (1994).

Mijn werk op het gebied van coordinaat-onafhankelijke representatie is vooral gebaseerd op de theorie van Backus en de multi-polen van Maxwell. Dit proefschrift bevat toepassingen en verdere ontwikkelingen van deze theorie. In de multi-pool formulering worden de stabiliteit condities van de drie-dimensionale tensor van vierde orde niet meegenomen. Een drie-dimensionale tensor van vierde orde die voldoet aan de symmetrie voorwaarden voor elastische tensoren wordt hier gedefinieerd als een hierarchisch symmetrische tensor (HST). Deze definitie bevat geen stabiliteit condities.

De theorie van Backus is gebaseerd op een specifieke decompositie van de HST in harmonische tensoren en de multi-polen van Maxwell zijn de geometrische voorstelling van de harmonische tensor in de 3-dimensionale ruimte. Deze voorstelling bestaat uit boeketten van 3-dimensionale vectoren plus twee skalars.

Hoofdstuk 1 geeft een beschrijving van eerder onderzoek gedaan naar decompositie van elastische tensoren. Het bevat in het bijzonder een terugblik op het multi-pool principe ontwikkelt door Maxwell (1881), de samenhang met sferische harmonischen en hoe ze gebruikt kunnen worden in de tensor analyse van elastische tensoren. Een belangrijk principe in de multi-pool formulering is dat van totale symmetrie. In een totaal symmetrische vierde orde tensor, T_{ijkl}, zijn alle tensor componenten met specifieke indices i, j, k , en l gelijk, ongeacht de permutaties van de indices. Een Corrigendum werd gepubliceerd door Cowin (1993) na een discussie over totale symmetrie.

In hoofdstuk 2 wordt totale symmetrie gebruikt en worden er numerieke voorbeelden gegeven. Eigenwaarde problemen worden opgelost door symmetrische coordinaten stelsels te vinden. Ook wordt er een vergelijking gemaakt tussen verschillende decomposities van de HST tensor.

Een basis van 21 orthonormale basis tensoren in de vector-ruimte van HST worden gedefinieerd in hoofdstuk 3. De basis tensoren worden afgeleid van sferische harmonischen. Een decompositie van de elasticiteit tensor in 21 basis tensoren voor verschillende symmetrie klassen wordt gepresenteerd.

In de tensor analyse worden principes van de moderne algebra toegepast. Moderne algebra, zoals groepentheorie, schijnt belangrijk te zijn voor de verdere ontwikkeling van de elastische anisotropie theorie.

In hoofdstuk 4 wordt een classificatie van symmetrie systemen gegeven door middel van de structuur van de vectoren in de boeketten, en de lengte van de boeketten van 3-dimensionale vectoren worden afgeleid. Er worden voorbeelden gegeven waarbij multi-polen worden getoond alsmede hun coordinaat-vrije eigenschap. De formules die de lengte beschrijven zijn geprogrammeerd in computer software en worden toegepast in hoofdstuk 6 waar verstoring wordt besproken.

Omdat de lengte van de vector nul wordt voor isotrope symmetrie, zou bij verdere ontwikkeling de lengte gebruikt kunnen worden als maat voor de afwijking van isotropie. Alleen de twee skalaren in de harmonische decompositie bepalen de twee onafhankelijke componenten van een tensor met isotrope symmetrie.

In de literatuur wordt de term "elastische tensor" meestal gebruikt voor tensoren met dimensie 3 en orde 4, die een reeel, d.w.z. een stabiel, medium beschrijven. De theorie van Backus is echter geldig ongeacht de stabiliteit conditie. Overeenkomstig de introductie van het begrip "hierarchisch symmetrische tensor", is dit gaandeweg steeds meer gebruikt in mijn werk (hoofdstukken 3, 4, 5 en 6). In mijn eerste publicatie (hoofstuk 2) zijn hierarchisch symmetrische tensoren echter niet gebruikt. Ik heb dat in mijn proefschrift zo gelaten, met uitzondering van kleine wijzigingen.

De interne structuur van de boeketten van 3-dimensionale vectoren die de multipolen definieren, zijn onafhankelijk van het coordinaten stelsel ten opzichte waarvan de tensor is gedefinieerd. Daarom zijn de richtingen van de vectoren en de lengte onafhankelijk van de orientatie van het coordinaten stelsel: d.w.z. de eigenschappen zijn coordinaat-onafhankelijk. Een ander voorbeeld van coordinaat-onafhankelijkheid is de structuur van eigenvectoren van tweede orde tensoren geassocieerd met HST. Verschillende tweede orde tensoren gerelateerd aan de elastische tensor zijn onderzocht op hun eigenvectoren, en een classificatie van eigenvectoren voor verschillende symmetrie systemen wordt gegeven in hoofdstuk 5.Voor monokline en hogere symmetrie bestaan er altijd eigenvectoren die samenvallen met symmetrie assen en normalen op de symmetrie vlakken. Het deviatorische gedeelte van de geanalyseerde tweede orde tensoren wordt nul voor kubische en isotrope symmetrie, en zou gebruikt kunnen worden om de afwijking van isotrope of kubische symmetrie te definieren.

Het meeste van mijn werk is gerelateerd aan ideale media, met symmetrie eigenschappen zoals in de kristal-fysica. In hoofdstuk 6 wordt het meten van echte data gemodelleerd door tensoren met ideale symmetrie te verstoren. Het verstoren van een tricline tensor modelleert het meten van onnauwkeurigheid.

Verstoring van een HST geeft aan of de multi-polen "stabiel" zijn. Een verstoring van vijf procent voor een bepaalde tensor met tricline symmetrie leidt ertoe dat de verschillende multi-polen ongeveer evenveel afwijken, gegeven de definitie van afwijking zoals ik die heb toegepast. De afwijkingen zijn 5.8%, 4.9% en 6.8% voor een speciaal gekozen vector in het boeket van respectievelijk $H^{(4)}$, en $H^{(2)}$ en $h^{(2)}$. Er wordt ook een voorbeeld gegeven van een tensor met orthorhombische symmetrie, waarbij getoond wordt hoeveel de symmetrie elementen veranderen ten gevolge van verstoring van de tensor.

Verstoring van een tensor met ideale hogere symmetrie modelleert de afwijking van ideale symmetrie. Verder werk op het gebied van toepassing van fundamentele principes is nodig om de mate van afwijking van ideale symmetrie te bepalen.

Theoretische analyse van elastische anisotropie heeft een veel groter toepassingsbereik dan alleen de aardwetenschappen, en komt ook voor in wetenschappen als wiskunde, natuurkunde, materiaalkunde en biomechanica.

Gedeelten van het werk zijn gepubliceerd als twee artikelen en een derde artikel is geaccepteerd en wordt gedrukt.

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Acknowledgements

The work on my thesis has been done partly at the University of Utrecht, and partly at Stavanger College where I have my permanent position. Professor Klaus Helbig has been my supervisor and promotor.

The work started at the University of Utrecht, and I appreciate very much the opportunity I had to stay there for two years. I would like to thank Professor emeritus Dr. K. Helbig for advice, discussions and encouragement. I am grateful for all his support during the work on my thesis. He is specifically thanked for the opportunity to use software developed by him.

In addition the following persons at mathematical institutes are thanked for fruitful discussions: Dr. W.L.J. van den Kallen at the University of Utrecht, Professor Dr. H. Tverberg at the University of Bergen, Dr. K. Ranestad at the University of Oslo. I would also like to thank my colleagues in Stavanger, and especially Dr. M. Dale for fruitful discussions, and referees for their comments in publishing.

Thanks also to Dr. Henk Hake for his translation of a summary into Dutch.

The first year in Utrecht was funded by a sabbatical from my employer in Stavanger, and my second year by Royal Norwegian Council for Scientific and Industrial Research. I appreciate the opportunity they gave me. In addition I would like to thank Rogaland Research Academy for their financial support.

During finishing my thesis, I visited the Edinburgh Anisotropy Group, British Geological Survey. I appreciate very much the opportunity to be there, and their help with the final draft.

Lastly I would like to thank my family and my friends for all their support and not at least their patience with me.

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