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MECHANICS

Tensor series expansion of a spherical function for the use in constitutive theory of materials containing orientable particles

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Abstract. This paper presents a didactical introduction to a tensor series expansion of a spherical function for the use in constitutive theory of materials containing orientable particles. In several application areas a function of two angles, e.g. an orientation (density) distribution function, is expanded into a series of symmetric irreducible tensors. This paper will explain this series expansion, starting with reviewing the representation of a function defined on a unit sphere in terms of spherical harmonics, which are a possible choice for a basis. Then, the connection between spherical harmonics and symmetric traceless tensors is explained. This is the basis for introducing and understanding orientation and alignment tensors as well as their connection to the orientation distribution function. The style of presentation was chosen to be more on the didactical side, differently from the theorem–proof style found elsewhere, which directly starts from symmetric tensors.

Key words: fibre orientation, tensor series, spherical surface harmonics, constitutive equations, alignment tensors, orientation tensors.

1. INTRODUCTION

In many materials like molecular gases [1, 2], liquid crystals [3–6], polymers, and short fibre reinforced materials [7–15] the orientation of the molecules or ‘particles’ plays an important role because different orientation distributions lead in general to different material properties. In liquid crystals, the optical properties depend on the orientation of the molecules; this can be used to change the polarization direction of light and is applied in liquid crystal displays. Examples for fibre reinforced materials include fibre reinforced plastics and fibre concrete. In short fibre reinforced concrete (SFRC), short steel fibres are added to the concrete in order to increase the tensile strength. There, great differences of stability are observed in dependence of the orientation of the fibres [16, 17].

Throughout this section it is assumed that the considered particles of the observed material are rigid and rod-like. Since the size of the particles is not necessary for indicating their orientation, one can assume that the particles have unit length without loss of information. Hence, the orientation of one particle can be specified by indication of the angles ϑ and φ (see Fig. 1).

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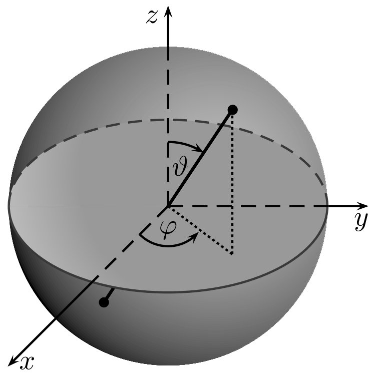


Fig. 1. The orientation of every particle is specified by the angles φ and ϑ.

The angles ϑ and φ, with $0 \leq \vartheta < \pi$ and $0 \leq \varphi < 2\pi$, can be used as coordinates on the surface of a unit-sphere. Therefore, the orientation of a fibre can be described as a point on a unit-sphere. If the two ends of a fibre are indistinguishable, each fibre orientation corresponds to two opposite points on the sphere.

With introducing a probability density f $\big($with $f(\vartheta,\varphi) \geq 0$ and $\oint f \mathrm{d}\Omega = 1$, where Ω is the surface element [18]$\big)$ it is possible to compute the probability that one particle is being situated in a specific area (see Fig. 2). In this context the probability density f is called orientation distribution function (ODF) (although it is not a probability distribution in mathematical sense!). The ODF gives complete information about the alignment of the considered particles and has influence on the material properties.

Examples of possible orientations of particles are shown in Fig. 3. In Fig. 3a the particles do not have a preferred orientation, thus the ODF is constant and with $\oint f \mathrm{d}\Omega = 1$ follows:

$$f(\vartheta,\varphi) = \frac{1}{4\pi}. \tag{1}$$

In Fig. 3b the density is given by

$$f(\vartheta,\varphi) = 1_{\{(0,2\pi)\times\{\pi/2\}\}}(\varphi,\vartheta) := \begin{cases} \frac{1}{2\pi} & ,\vartheta = \pi/2 \\ 0 & ,\text{else} \end{cases} , \tag{2}$$

which again follows from the condition $\oint f \mathrm{d}\Omega = 1$.

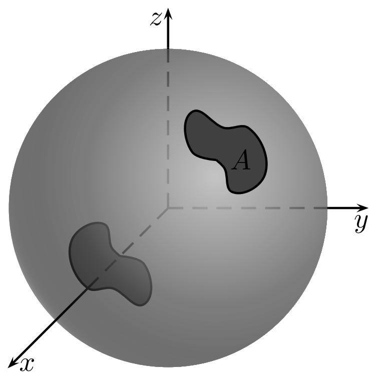
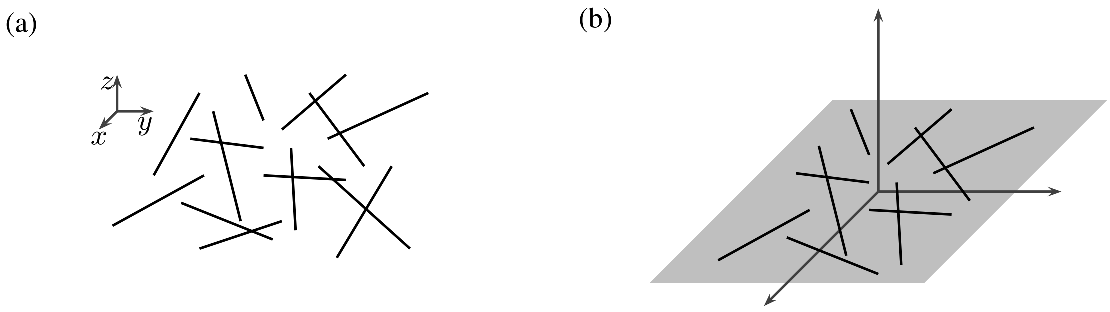


Fig. 2. The probability that particles are located in the area A is $P(A) := \oint_A f \mathrm{d}\Omega$.



No preferred orientation

All particles lie in one plane

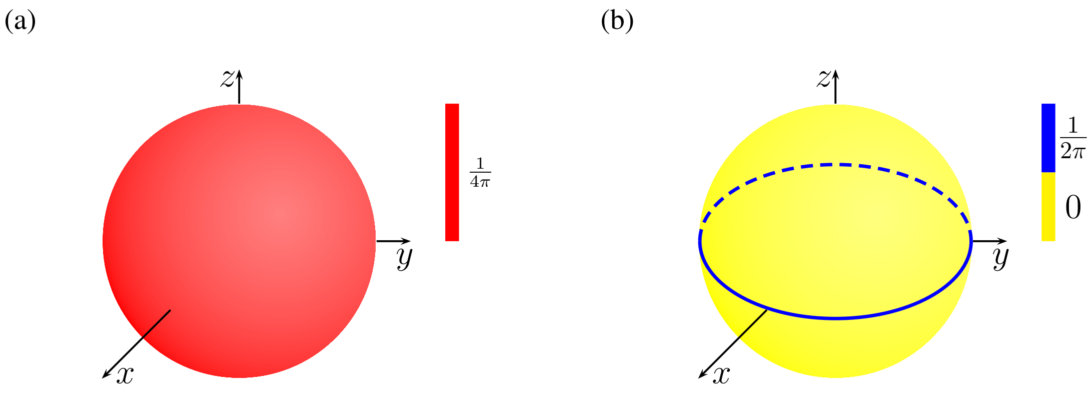
Fig. 3. Examples of orientation distributions.

The distribution functions can be visualized by plotting a coloured sphere, where for every $0 \leq \vartheta < \pi$ and $0 \leq \varphi < 2\pi$ the colour of the point $(\cos\varphi \sin\vartheta, \sin\varphi \sin\vartheta, \cos\vartheta)$ represents the value of $f(\vartheta, \varphi)$ (see Fig. 4). Every ODF f is dependent on the angles ϑ and φ and defined on the sphere $S^2 := \{\boldsymbol{x} \in \mathbb{R}^3 | \|x\| = 1\}$. In analogy to Fourier series, where a function is dependent on one angle φ or 2π-periodic resp. it is possible to express the ODF f in a (generally infinite) sum of 'spherical harmonics', where the spherical harmonics are the two-dimensional analogues to the sines and cosines in the Fourier series (see Section 2). Hence, with denoting Y_l^m as spherical harmonics for $l \in \mathbb{N}_0$, $|m| \leq l$, we can express the ODF as the series

$$f(\vartheta, \varphi) \quad = \quad \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \alpha_{lm} Y_l^m(\vartheta, \varphi) \tag{3}$$

with suitable chosen real coefficients α_{lm}. With $\boldsymbol{n} = (\cos\varphi \sin\vartheta, \sin\varphi \sin\vartheta, \cos\vartheta)$, $f(\boldsymbol{n}) := f(\vartheta, \varphi)$, and $Y_l^m(\boldsymbol{n}) := Y_l^m(\vartheta, \varphi)$, we obtain the equivalent cartesian expression

$$f(\boldsymbol{n}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \alpha_{lm} Y_l^m(\boldsymbol{n}). \tag{4}$$



Plot of ODF of Fig. 3a. No preferred orientation (isotropic)

Plot of ODF of Fig. 3b. All particles oriented within one plane, but no preference within this plane

Fig. 4. Visualization of the ODF given in Fig. 3.

However, for many applications it has been proven worthwhile to use a tensorial description instead of expressing f in a series of spherical harmonics. This means that the ODF can be expanded into a series using tensor coefficients $a_{\mu_1 \ldots \mu_l}$; the cartesian expansion is given in the following way [1,19–21]:

$$f(\boldsymbol{n}) \quad = \quad \frac{1}{4\pi}\left(1+\sum_{l=1}^{\infty}\frac{(2l+1)!!}{l!}a_{\mu_1\ldots\mu_l}n_{\mu_1}\cdots n_{\mu_l}\right), \tag{5}$$

$$a_{\mu_1\ldots\mu_l} \quad = \quad \oint_{S^2} f(\boldsymbol{n})\ \overline{n_{\mu_1}\cdots n_{\mu_l}}\ d^2n, \tag{6}$$

where $\overline{n_{\mu_1}\cdots n_{\mu_l}}$ is the symmetric traceless part of the l-fold tensor product of $\boldsymbol{n}$ with itself (see Appendix A, Definition 4 and Section 3). The !! denotes a factorial with double steps and the μ_i are the vector indices, $\mu_i = 1,2,3,\ i = 0,\ldots,l$.

In Eq. (5) the Einstein summation convention is used; thus, every index that appears twice on the right side of Eq. (5) implies summation over all values of the index, i.e. the right term of Eq. (5) is equivalent to

$$\frac{1}{4\pi}\left(1+\sum_{l=1}^{\infty}\sum_{\mu_1,\cdots,\mu_l=1}^{3}\frac{(2l+1)!!}{l!}a_{\mu_1\ldots\mu_l}n_{\mu_1}\cdots n_{\mu_l}\right). \tag{7}$$

For better understanding of the notation of the formula we explicitly write down the first few terms of the series in Eq. (5):

$$f(\boldsymbol{n}) \quad = \quad \frac{1}{4\pi}\left(1+\sum_{\mu_1=1}^{3}\frac{(2\cdot 1+1)!!}{1!}a_{\mu_1}n_{\mu_1}+\sum_{\mu_1,\mu_2=1}^{3}\frac{(2\cdot 2+1)!!}{2!}a_{\mu_1\mu_2}n_{\mu_1}n_{\mu_2}+\cdots\right), \tag{8}$$

$$\quad = \quad \frac{1}{4\pi}\left(1+3a_{\mu_1}n_{\mu_1}+\frac{5\cdot 3}{2}a_{\mu_1\mu_2}n_{\mu_1}n_{\mu_2}+\cdots\right). \tag{9}$$

Example 1. In this example the second-order alignment tensor of the flat distribution from Fig. 4b is calculated. For simplicity a discrete distribution of only two fibres is considered. These fibres have the orientations $(\vartheta,\varphi) = (90°,0°)$ and $(\vartheta,\varphi) = (90°,90°)$.

The first step is to convert the orientations from spherical polar coordinates to cartesian coordinates:

$$\boldsymbol{n}^{<1>} \quad = \quad \begin{pmatrix}1\\0\\0\end{pmatrix} \quad , \quad \boldsymbol{n}^{<2>} \quad = \quad \begin{pmatrix}0\\1\\0\end{pmatrix}. \tag{10}$$

The next step is to calculate the alignmen tensor using Eq. (6):

$$\mathbf{a} \quad = \quad \oint_{S^2} f(\boldsymbol{n})\ \overline{\boldsymbol{n}\otimes\boldsymbol{n}}\ d^2n = \frac{1}{N}\sum_{i}^{N}\boldsymbol{n}^{<i>}\otimes\boldsymbol{n}^{<i>}-\frac{1}{3}\mathbf{1}\,. \tag{11}$$

To do this, the sum of outer products of the orientations of the two fibres is calculated

$$\frac{1}{N}\begin{pmatrix}1\\0\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\\0\end{pmatrix}+\frac{1}{N}\begin{pmatrix}0\\1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\\0\end{pmatrix} \quad = \quad \frac{1}{2}\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix}+\frac{1}{2}\begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix}, \tag{12}$$

and then, with removing the trace, the second-order alignment tensor results in

$$a_{\mu\nu} \quad = \quad \frac{1}{2}\begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix}-\frac{1}{3}\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix} = \begin{pmatrix}\frac{1}{6}&0&0\\0&\frac{1}{6}&0\\0&0&-\frac{1}{3}\end{pmatrix}. \tag{13}$$

Comparing the second-order alignment tensor just calculated with the one presented in Eq. (111) in Appendix B, one can see that the flat isotropic distribution is approximated in the first order using the spherical harmonic $-Y_2^0$. □

The equivalence of Eq. (5) and Eq. (4) will be shown in two steps. First, a series expansion of the ODF into spherical harmonics will be performed (Section 2); second, after a short introduction to symmetric irreducible tensors (Section 3), the correspondence of symmetric irreducible tensors with spherical harmonics will be shown (Section 4).

2. SERIES EXPANSION USING SPHERICAL HARMONICS

2.1. Function spaces as vector spaces

The first thing to understand is that also functions can form a vector space. The definition of a vector space is repeated for completeness in Definition 6 in Appendix A. In the following we only consider function spaces where functions map from an arbitrary non-empty set D into a vector space V over the field F (for the reader unfamiliar with the notion 'field' it is for our purposes sufficient to replace F with $\mathbb{R}$ or $\mathbb{C}$). We notate these function spaces as $F(D,V)$, i.e. $F(D,V)$ is the set of all functions that map from D to V.

The function space $F(D,V)$ becomes a vector space if we endow the space with an addition and scalar multiplication such that the vector space axioms in Definition 6 are fulfilled. For $\lambda \in F$ and the functions $f,g : D \to V$ we define the addition $f+g$ and scalar multiplication λf by

$$f+g \quad : \quad D \to V, x \mapsto (f+g)(x) := f(x)+g(x), \tag{14}$$
$$\lambda f \quad : \quad D \to V, x \mapsto (\lambda f)(x) := \lambda \cdot f(x). \tag{15}$$

Note that the operations + and $\cdot$ in the terms $f(x)+g(x)$ and $\lambda \cdot f(x)$ refer to the already defined operations in the vector space V since $f(x), g(x)$ are vectors in V for every $x \in D$. With this in mind it can be easily shown that the set $F(D,V) = \{f : D \to V\}$ will become a vector space if endowed with the operations + and $\cdot$ defined in Eq. (14) and Eq. (15). Although it might be at first sight unfamiliar to consider a function as a vector and a function space as a vector space, this approach allows us to use all the results that have been proved for general vector spaces.

2.2. Scalar product and orthogonal system

The canonical scalar product in $\mathbb{R}^n$ is defined by $x \cdot y := \langle x,y \rangle := x_i y_i$ (using the Einstein sum convention) for every $x,y \in \mathbb{R}^n$. Two vectors x,y are called orthogonal if $\langle x,y \rangle = 0$ and the norm of $x \in \mathbb{R}^n$ is defined by $\|x\| := \sqrt{\langle x,x \rangle}$. Again it is possible to generalize these notions and define a scalar product and a norm on any vector space. The definitions of a scalar product and norm in an arbitrary vector space are repeated in Definition 7 and Definition 8, respectively, in Appendix A.

For our purposes we consider the function space $F(D,V) := F(S^2,\mathbb{R})$ and define a scalar product by

$$\langle f,g \rangle := \int_{S^2} f(x)g(x)\mathrm{d}x. \tag{16}$$

As the functions are real-valued, the complex conjugation of the first function under the integral is omitted. It is a useful exercise for the reader to check that Definition 7 is fulfilled. A norm is induced by the scalar product, i.e.

$$\|f\| := \sqrt{\langle f,f \rangle}. \tag{17}$$

For the further development some more notions with regard to the functionspace $F(S^2,\mathbb{R})$ will be introduced.

Definition 1. *The space $L^2(S^2)$ of square integrable functions on $S^2 = \{\boldsymbol{x} \in \mathbb{R}^3 | \|x\| = 1\}$ is defined by*

$$L^2(S^2) := \left\{ f \in F(S^2, \mathbb{R}) \middle| \|f\| < \infty \right\}. \tag{18}$$

As a note, the space $L^2(S^2)$ is a Hilbert space, meaning it is a vector space with a scalar product that is complete with respect to the norm induced by the scalar product.

Definition 2 (Schauder basis)**.** *A* Schauder basis *is a set of functions $\{g_1, g_2, \dots\}$ in $L^2(S^2)$ such that for every function $f \in L^2(S^2)$ there exists a unique sequence of real coefficients $\alpha_1, \alpha_2, \dots$ so that*

$$f = \sum_{i=1}^{\infty} \alpha_i g_i \,. \tag{19}$$

Note that a Schauder basis does not need to be a vector space basis (Hamel basis) because we allow infinite linear combinations (whereas in a vector space basis every vector can be represented as a finite linear combination of basis vectors).

Definition 3. *The set $\{g_1, g_2, \dots\}$ is called an orthonormal system (ONS) if*

$$\langle g_i, g_j \rangle = \delta_{ij}.$$

If $\{g_1, g_2, \dots\}$ is both a Schauder basis and an ONS, it holds [22]

$$f = \sum_{i=1}^{\infty} \langle f, g_i \rangle g_i \,, \tag{20}$$

i.e. every coefficient α_i in Eq. (19) is given by $\alpha_i = \langle f, g_i \rangle$.

2.3. Spherical harmonics

The three-dimensional Laplace operator in spherical coordinates is given by [18]

$$\Delta_3 \;=\; \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)}_{=:\Delta_r \text{ , radial part}} + \underbrace{\frac{1}{r^2}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right]}_{=:\Delta_{\vartheta,\varphi} \text{ , angular part}}. \tag{21}$$

Scalar functions $Y : S^2 \to \mathbb{R}$ are denoted as *spherical harmonics* if they solve the angular part of the 3-dimensional Laplace equation $\Delta_3 \Psi = 0$, i.e. a separation of variables is performed for $\Psi(r, \vartheta, \varphi) = F(r)Y(\vartheta, \varphi)$:

$$0 \;=\; \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) F(r)Y(\vartheta,\varphi) + \frac{1}{r^2}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right] F(r)Y(\vartheta,\varphi). \tag{22}$$

For us, only the spherical part is of interest.

It can be shown that for $l \in \mathbb{N}_0, m \in \{-l, -l+1, \dots, 0, \dots, l-1, l\}$ the functions $Y_l^m : (0, 2\pi) \times (0, \pi) \longrightarrow \mathbb{R}$,

$$Y_l^m(\varphi, \vartheta) = N_{(l,|m|)} P_l^{|m|}(\cos\vartheta) \cdot \begin{cases} \cos(m\varphi) & , 1 \le m \le l \\ \frac{1}{2} & , m = 0 \\ \sin(|m|\varphi) & , -l \le m \le -1 \end{cases} \tag{23}$$

are spherical harmonics, where P_l^m is given by

$$P_l^m(x) = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l \ , \tag{24}$$

and the short form $N_{(l,m)}$ is defined as $N_{(l,m)} := \sqrt{\frac{(2l+1)}{2\pi}\frac{(l-m)!}{(l+m)!}}$.

With the scalar product defined in Eq. (16) the spherical harmonics are orthonormal, i.e.

$$\langle Y_l^m, Y_k^n \rangle = \int_{S^2} Y_l^m Y_k^n dn = \delta_{lk}\delta_{mn}. \tag{25}$$

Furthermore, the set of all spherical harmonics forms a Schauder basis of L^2 and therefore it is possible to expand the ODF into a series of spherical harmonics

$$f(\boldsymbol{n}) \quad = \quad \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \alpha_{lm} Y_l^m(\boldsymbol{n}) \tag{26}$$

with the coefficients

$$\alpha_{lm} \quad = \quad \langle f(\boldsymbol{n}), Y_l^m(\boldsymbol{n})\rangle. \tag{27}$$

In Table 1 the first few real spherical harmonics are displayed and in Table 2 the spherical harmonics of Table 1 are visualized.

3. SYMMETRIC TRACELESS TENSORS

In this section we give a short introduction to symmetric traceless tensors and define a function space H_l that is connected with these tensors, which is, as we will see in Section 4, equal to $\text{span}_{m\leq l} Y_l^m$. We start with a short description of tensors and the notations used in this article. The reader unfamiliar with tensors can find a more detailed introduction in Ref. [23].

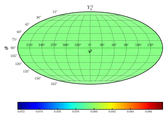
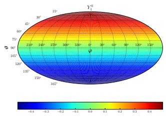
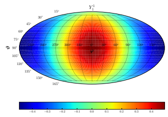
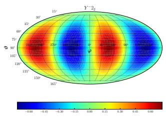
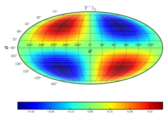
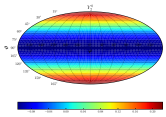
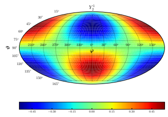
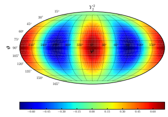
A tensor in general is a multicomponent quantity, whereby the realvalued components are dependent on the chosen coordinate system. A tensor is of the lth order if its components can be indexed by l integers $\mu_1,\ldots,\mu_l$; thus, to give an example, a zeroth-, first-, or second-order tensor can be represented by a scalar, vector, or matrix, respectively. We denote with $[a_{\mu_1\ldots\mu_l}]$ a tensor of the lth order itself and with $a_{\mu_1\ldots\mu_l}$ we refer to the components of the tensor with regard to the chosen basis.

We give now a short introduction to the notions *symmetric* and *traceless* and illustrate these for tensors of the order $l = 0,1,2$.

Table 1. The spherical harmonics for $l = 0,1,2$

	$l=0$	$l=1$	$l=2$
$m=-2$			$\sqrt{\frac{45}{28\pi}}\sin^2\vartheta\sin(2\varphi)$
$m=-1$		$\sqrt{\frac{3}{4\pi}}\sin\vartheta\sin\varphi$	$-\sqrt{\frac{15}{4\pi}}\sin\vartheta\cos\vartheta\sin\varphi$
$m=0$	$\frac{1}{4\pi}$	$\sqrt{\frac{3}{4\pi}}\cos\vartheta$	$\sqrt{\frac{5}{128\pi}}(3\cos^2\vartheta-1)$
$m=1$		$\sqrt{\frac{3}{4\pi}}\sin\vartheta\cos\varphi$	$-\sqrt{\frac{15}{4\pi}}\sin\vartheta\cos\vartheta\cos\varphi$
$m=2$			$\sqrt{\frac{45}{28\pi}}\sin^2\vartheta\cos(2\varphi)$

Table 2. Visualization of the spherical harmonics of Table 1 using a 'Mollweide' projection

	$m=-2$	$m=-1$	$m=0$	$m=1$	$m=2$
$l=0$					
$l=1$					
$l=2$					

A tensor $[a_{\mu_1\ldots\mu_l}]$ is called *symmetric* provided

$$a_{\mu_1\ldots\mu_l} = a_{\eta_1\ldots\eta_l}, \tag{28}$$

where $\eta_1\ldots\eta_l$ is any reordering of the indices $\mu_1\ldots\mu_l$. For tensors of the order 0 or 1 this is not a restriction, since we have zero or one index, respectively, which we cannot permutate. For $l=2$ a tensor is symmetric if

$$a_{ij} = a_{ji}. \tag{29}$$

A tensor $[a_{\mu_1\ldots\mu_l}]$ is called *traceless* if the sum over any two indices that are set equal to each other is zero. Thus, if we consider the indices $\mu_1\ldots j\ldots j\ldots\mu_l$, this yields

$$0 = a_{\mu_1\ldots j\ldots j\ldots\mu_l} = \sum_{j=1}^{3} a_{\mu_1\ldots j\ldots j\ldots\mu_l}. \tag{30}$$

For symmetric tensors this condition reduces to

$$a_{jj\mu_3\ldots\mu_l} = 0,$$

since the ordering of the indices does not make any difference. Tensors of the order 0 or 1 are defined as always being traceless. A tensor of the order $l=2$ is traceless provided

$$a_{jj} = a_{11} + a_{22} + a_{33} = 0. \tag{31}$$

It is often useful to decompose a tensor into a sum of 'special' tensors and to consider only several parts of the decomposition. For our purpose we decompose every tensor into a symmetric and a skewsymmetric part, whereby a tensor $[a_{\mu_1\ldots\mu_l}]$ is called skewsymmetric if all the components $a_{\mu_1\ldots\mu_l}$ change its sign under the exchange of any pair of its indices, i.e. for example the following holds:

$$a_{\mu_1\mu_2\mu_3\ldots\mu_l} = -a_{\mu_2\mu_1\mu_3\ldots\mu_l}. \tag{32}$$

For the sake of comprehension we consider again the zeroth-, first-, and second-order tensors. Tensors of the order zero and one are per definition symmetric traceless and have no skewsymmetric part. A second-order tensor $[a_{ij}]$ in $\mathbb{R}^3$ can be represented as a matrix (a_{ij})

$$(a_{ij}) = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \tag{33}$$

and has the decomposition

$$(a_{ij}) = \underbrace{\begin{pmatrix} a_{11} & \frac{a_{12}+a_{21}}{2} & \frac{a_{13}+a_{31}}{2} \\ \frac{a_{12}+a_{21}}{2} & a_{22} & \frac{a_{23}+a_{32}}{2} \\ \frac{a_{13}+a_{31}}{2} & \frac{a_{23}+a_{32}}{2} & a_{33} \end{pmatrix}}_{:=[a_{ij}]^{\mathrm{Sym}} \,=\, \text{symmetric}} + \underbrace{\begin{pmatrix} 0 & \frac{a_{12}-a_{21}}{2} & \frac{a_{13}-a_{31}}{2} \\ -\frac{a_{12}-a_{21}}{2} & 0 & \frac{a_{23}-a_{32}}{2} \\ -\frac{a_{13}-a_{31}}{2} & -\frac{a_{23}-a_{32}}{2} & 0 \end{pmatrix}}_{\text{skewsymmetric}}, \tag{34}$$

where $\mathrm{tr}(A) = a_{ii} = a_{11} + a_{22} + a_{33}$ is the trace of the tensor $[a_{ij}]$.

The symmetric part $[a_{ij}]^{\mathrm{Sym}}$ can be further decomposed into a traceless symmetric and isotropic part

$$(a_{ij})^{\mathrm{Sym}} = \underbrace{\begin{pmatrix} a_{11} - \frac{1}{3}\,\mathrm{tr}(A) & \frac{a_{12}+a_{21}}{2} & \frac{a_{13}+a_{31}}{2} \\ \frac{a_{12}+a_{21}}{2} & a_{22} - \frac{1}{3}\,\mathrm{tr}(A) & \frac{a_{23}+a_{32}}{2} \\ \frac{a_{13}+a_{31}}{2} & \frac{a_{23}+a_{32}}{2} & a_{33} - \frac{1}{3}\,\mathrm{tr}(A) \end{pmatrix}}_{:=\overline{a_{ij}} \,=\, \text{traceless symmetric}} + \underbrace{\begin{pmatrix} \frac{1}{3}\,\mathrm{tr}(A) & 0 & 0 \\ 0 & \frac{1}{3}\,\mathrm{tr}(A) & 0 \\ 0 & 0 & \frac{1}{3}\,\mathrm{tr}(A) \end{pmatrix}}_{\text{isotropic}}. \tag{35}$$

Every tensor $[a_{\mu_1\cdots\mu_l}]$ can be decomposed in this way. A recursive formula for the computation of the symmetric traceless part $\overline{a_{\mu_1\cdots\mu_l}}$ can be found in Ref. [20].

The set of all symmetric traceless tensors

$$\begin{aligned} V_l : &= \{[a_{\mu_1\cdots\mu_l}] | [a_{\mu_1\cdots\mu_l}] \text{ is of the } l\text{th order, symmetric and traceless } \} \\ &= \{ \overline{a_{\mu_1\cdots\mu_l}} \, | [a_{\mu_1\cdots\mu_l}] \text{ is a tensor a of } l\text{-th order}\} \end{aligned} \tag{36}$$

forms a vector space; hence, V_l has a dimension N and a basis $\{[b^1], \ldots, [b^N]\}$ such that every symmetric traceless tensor can be expressed as a linear combination of the tensors $[b^1], \ldots, [b^N]$.

In order to determine the dimension of V_l we consider as an example the dimension of the vector spaces V_0, V_1, and V_2.

Every tensor $[a] \in V_0$ is a scalar and we have therefore $\dim V_0 = 1$. The first-order tensors $[a_i] \in V_1$ have three components: a_1, a_2, and a_3. As every first-order tensor is symmetric traceless, the components a_1, a_2, and a_3 are linearly independent, which yields $\dim V_1 = 3$.

Every $[a_{ij}] \in V_2$ has nine components $a_{11}, a_{12}, \ldots, a_{33}$. These components can not all be chosen arbitrarily because the tensor has to be symmetric and traceless. It turns out that if we have for example chosen the five components $a_{11}, a_{12}, a_{13}, a_{22}$, and a_{23}, the tensor is already completely defined by the conditions $a_{21} = a_{12}, a_{31} = a_{13}, a_{32} = a_{23}$, and $a_{33} = -a_{11} - a_{22}$. Hence the dimension of V_2 is

$$\dim V_2 = 5\,, \tag{37}$$

and we can find a basis $B_2 = \{[b^1], \ldots, [b^5]\}$ such that every symmetric traceless tensor $[a_{ij}] \in V_2$ can be expressed as a linear combination of the basis elements.

In general the dimension of V_l is

$$\dim V_l = 2l + 1, \tag{38}$$

which is shown in Ref. [20].

Now we define the function space H_l based on traceless symmetric tensors. For better viewing we use in the following the short form $[a] := [a_{\mu_1\ldots\mu_l}] \in V_l$ for traceless symmetric tensors.

We define with

$$h_{l,[a]} := \begin{cases} S^2 \longrightarrow \mathbb{R} \\ \boldsymbol{n} = (n_1, n_2, n_3) \longmapsto a_{\mu_1\ldots\mu_l} n_{\mu_1} \ldots n_{\mu_l} \end{cases} \tag{39}$$

the function space

$$H_l := \left\{ h_{l,[a]} \middle| [a] = [a_{\mu_1\ldots\mu_l}] \in V_l \right\}. \tag{40}$$

Note that again in Eq. (39) Einstein's summation convention is used, i.e.

$$h_{l,[a]}(\boldsymbol{n}) = \sum_{\mu_1\ldots\mu_l=1}^{3} a_{\mu_1\ldots\mu_l} n_{\mu_1} \ldots n_{\mu_l}. \tag{41}$$

The function space H_l becomes a vector space if endowed with the operations + and $\cdot$ defined in Eq. (14) and Eq. (15). With $\dim V_l = 2l+1$ we obtain $\dim H_l = 2l+1$ and for a basis $\{[b^1], \ldots, [b^{2l+1}]\}$ of V_l the functions $\left\{ h_{l,[b^1]}, \ldots, h_{l,[b^{2l+1}]} \right\}$ form a basis of H_l.

4. SYMMETRIC TRACELESS TENSORS AS SPHERICAL HARMONICS

The three-dimensional Laplace operator in spherical coordinates is given in Eq. (21). We denote

$$\Delta_{\vartheta,\varphi} := \frac{1}{r^2} \left[\frac{1}{\sin\vartheta} \frac{\partial}{\partial\vartheta} \left(\sin\vartheta \frac{\partial}{\partial\vartheta} \right) + \frac{1}{\sin^2\vartheta} \frac{\partial^2}{\partial\varphi^2} \right] \tag{42}$$

as the angular part of the Laplace operator ($\Delta_{\vartheta,\varphi}$ is also denoted as the Laplace–Beltrami operator in [20]). The operator $\Delta_{\vartheta,\varphi}$ has the eigenvalues $-l(l+1)$ for $l \in \mathbb{N}_0$ with eigenfunctions Y_l^m ($|m| \leq l$), i.e.

$$\Delta_{\vartheta,\varphi} \, Y_l^m(\vartheta,\varphi) \quad = \quad -l(l+1) Y_l^m(\vartheta,\varphi). \tag{43}$$

The eigenspace of the eigenvalue $-l(l+1)$ is defined by

$$\mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)} := \{\Phi \in L^2(S^2) | \Delta_{\vartheta,\varphi}\Phi = -l(l+1)\Phi\}. \tag{44}$$

Note that with Eq. (43) every linear combination of spherical harmonics of the lth order is an eigenfunction of $\Delta_{\vartheta,\varphi}$, therefore we have

$$\operatorname*{span}_{m\leq l} Y_l^m \subseteq \mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)} \; . \tag{45}$$

The Y_l^m are a set of orthogonal functions. For fixed l there are $2l+1$ orthogonal Y_l^m, $\mathrm{span}_{m\leq l} Y_l^m$ is therefore $(2l+1)$-dimensional. The dimension of the eigenspace of $\Delta_{\vartheta,\varphi}$ for the fixed eigenvalue $-l(l+1)$ is also $2l+1$. Looking at the dimensions of the spaces $\mathrm{span}_{m\leq l} Y_l^m$ and $\mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)}$ and at Eq. (45), one can argue that the spaces are equal. Therefore, it is shown that $\mathrm{span}_{m\leq l} Y_l^m$ is not only a subset of $\mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)}$, but the spaces are equal, i.e.

$$\operatorname*{span}_{m\leq l} Y_l^m = \mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)}. \tag{46}$$

The eigenspace $\mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)}$ is a $2l+1$-dimensional vector space. One possible basis is the set of the spherical harmonics $\{Y_l^{-l}, Y_l^{-l+1}, \ldots, Y_l^{l-1}, Y_l^{l}\}$ and every eigenfunction is a linear combination of spherical harmonics.

The aim is now to prove that

$$\operatorname*{span}_{m\leq l} Y_l^m = H_l, \tag{47}$$

because then every spherical hamonic can be expressed as a linear combination of functions h_l, which are defined in Eq. (39), such that we can replace the spherical harmonics in the series expansion in Eq. (4) by symmetric traceless tensors, which leads to Eq. (5).

We obtain Eq. (47) if and only if

$$\mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)} = H_l. \tag{48}$$

In order to show Eq. (48), we have to prove that

$$\Delta_{\vartheta,\varphi}\, h_{l,[a]} = -l(l+1)h_{l,[a]} \tag{49}$$

holds for all $h_{l,[a]} \in H_l$. For this, we extend first of all the range of the definition of the functions $h_{l,[a]}$ and define

$$\tilde{h}_{l,[a]} := \begin{cases} \mathbb{R}^3 \to \mathbb{R} \\ x = (x_1, x_2, x_3) \mapsto a_{\mu_1\ldots\mu_l} x_{\mu_1} \ldots x_{\mu_l} \end{cases}, \tag{50}$$

where again $[a]$ is a symmetric traceless tensor of the order l. For every $l \in \mathbb{N}$ the functions $\tilde{h}_{l,[a]}$ are harmonic, i.e.

$$\Delta \tilde{h}_{l,[a]} = 0, \tag{51}$$

which we will demonstrate for $l = 0, 1$, and 2. The proof for the general case is given in [20].

For $l = 0$ the tensor $[a]$ is a scalar, which yields

$$\Delta \tilde{h}_{0,[a]}(\boldsymbol{x}) = \Delta a = 0, \tag{52}$$

since the derivative of the constant $a \in \mathbb{R}$ vanishes.

For $l = 1$ the tensor $[a]$ is a vector and we obtain

$$\Delta \tilde{h}_{1,[a]}(\boldsymbol{x}) = \Delta a_i x_i = 0, \tag{53}$$

because the second derivative of $a_i x_i$ vanishes.

Using that the second-order tensor $[a]$ is traceless we finally obtain for $l = 2$

$$\begin{aligned} \Delta \tilde{h}_{2,[a]}(\boldsymbol{x}) &= \sum_{m=1}^{3} \frac{\partial}{\partial x_m}\frac{\partial}{\partial x_m} \sum_{\mu_1,\mu_2=1}^{3} a_{\mu_1\mu_2} x_{\mu_1} x_{\mu_2} \\ &= a_{\mu_1\mu_2} \frac{\partial}{\partial x_m}\frac{\partial}{\partial x_m}(x_{\mu_1}x_{\mu_2}) \\ &= a_{\mu_1\mu_2} \frac{\partial}{\partial x_m}(\delta_{\mu_1 m} x_{\mu_2} + \delta_{\mu_2 m} x_{\mu_1}) \\ &= a_{\mu_1\mu_2}(\delta_{\mu_1 m}\delta_{\mu_2 m} + \delta_{\mu_2 m}\delta_{\mu_1 m}) \\ &= 2\delta_{\mu_1\mu_2} a_{\mu_1\mu_2} = 2a_{\mu_1\mu_1} \underset{\substack{\uparrow \\ \text{traceless}}}{=} 0. \end{aligned} \tag{54}$$

With Eq. (51) it is now possible to prove Eq. (49).

For every vector $\boldsymbol{x} \in \mathbb{R}^3$ exist uniquely determined angles $\varphi \in [0, 2\pi), \vartheta \in [0, \pi)$, and $r \geq 0$ such that

$$\boldsymbol{x} = r(\cos\varphi \sin\vartheta, \sin\varphi \sin\vartheta, \cos\vartheta) \tag{55}$$

and with Eq. (55) we can write $\tilde{h}_{l,[a]}$ in spherical coordinates

$$\tilde{h}_{l,[a]}(r, \vartheta, \varphi) := \tilde{h}_{l,[a]}(\boldsymbol{x}). \tag{56}$$

Using Eqs (21), (56), and (51) leads then to

$$0 = \Delta_{\vartheta,\varphi}\, \tilde{h}_{l,[a]}(r, \vartheta, \varphi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\tilde{h}_{l,[a]}(r, \vartheta, \varphi)\right) + \frac{1}{r^2}\Delta_{\vartheta,\varphi}\, \tilde{h}_{l,[a]}(r, \vartheta, \varphi). \tag{57}$$

With $h_{l,[a]}(\vartheta, \varphi) := h_{l,[a]}(\cos\varphi \sin\vartheta, \sin\varphi \sin\vartheta, \cos\vartheta)$ holds

$$\tilde{h}_{l,[a]}(r, \vartheta, \varphi) = r^l h_{l,[a]}(\vartheta, \varphi), \tag{58}$$

which simply follows from the definition of the functions $h_{l,[a]}$ and $\tilde{h}_{l,[a]}$.

Thus, with inserting Eq. (58) in Eq. (57) we obtain

$$0 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} r^l h_{l,[a]}(\vartheta, \varphi)\right) + \frac{1}{r^2} r^l \Delta_{\vartheta,\varphi}\, h_{l,[a]}(\vartheta, \varphi). \tag{59}$$

Differentiation and excluding the term r^{l-2} yields

$$0 = r^{l-2}\bigg(l(l+1)h_{l,[a]}(\vartheta, \varphi) + \Delta_{\vartheta,\varphi}\, h_{l,[a]}(\vartheta, \varphi)\bigg), \tag{60}$$

which leads to

$$0 = l(l+1)h_{l,[a]}(\vartheta, \varphi) + \Delta_{\vartheta,\varphi}\, h_{l,[a]}(\vartheta, \varphi), \tag{61}$$

and we finally obtain

$$\Delta_{\vartheta,\varphi}\, h_{l,[a]}(\vartheta, \varphi) = -l(l+1)h_{l,[a]}(\vartheta, \varphi). \tag{62}$$

Thus, every function $h_{l,[a]} \in H_l$ is an eigenfunction of the operator $\Delta_{\vartheta,\varphi}$ with the eigenvalue $-l(l+1)$, which yields

$$H_l \subseteq \mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)}. \tag{63}$$

Since both the eigenspace $\mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)}$ and H_l are $2l+1$ dimensional, it holds

$$\mathrm{Eig}(\Delta_{\vartheta,\varphi})_{-l(l+1)} = H_l \tag{64}$$

and we obtain with Eq. (44)

$$\operatorname*{span}_{m \leq l} Y_l^m = H_l. \tag{65}$$

Hence, we can find for every spherical harmonic Y_l^m one particular symmetric traceless tensor $[a^{m,l}] \in V_l$ such that $h_{l,[a^{m,l}]} = Y_l^m$. The corresponding tensors $[a^{l,m}] \in V_l$ for $l \in \{0, 1, 2\}, |m| \leq l$ are explicitly specified in Appendix B.

To obtain the series expansion in Eq. (5) we first consider

$$\sum_{m=-l}^{l} \alpha_{l,m} Y_l^m(\boldsymbol{n}) = \underbrace{\sum_{m=-l}^{l} \alpha_{l,m} a^{m,l}_{\mu_1 \ldots \mu_l}}_{=: \tilde{a}_{\mu_1 \ldots \mu_l}} n_{\mu_1} \ldots n_{\mu_l} = \tilde{a}_{\mu_1 \ldots \mu_l} n_{\mu_1} \ldots n_{\mu_l}. \quad (66)$$

With Eq. (66) and

$$a_{\mu_1 \ldots \mu_l} := \frac{l!}{(2l+1)!!} \tilde{a}_{\mu_1 \ldots \mu_l}$$

we can then rewrite Eq. (4) as

$$f(\boldsymbol{n}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \alpha_{l,m} Y_l^m(\boldsymbol{n}) = \sum_{l=0}^{\infty} \frac{(2l+1)!!}{l!} a_{\mu_1 \ldots \mu_l} n_{\mu_1} \ldots n_{\mu_l}. \quad (67)$$

Hence, the tensorial description in Eq. (5) and the description using spherical harmonics in Eq. (4) are equivalent. The coefficients $a_{\mu_1 \ldots \mu_l}$ can be computed with formula (6), which is shown in Ref. [20].

5. ORIENTATION TENSORS, ALIGNMENT TENSORS, AND ORDER PARAMETERS

In the literature about materials containing fibres, the terms *orientation tensor* and *alignment tensor* appear frequently; in liquid crystal theory, an *order parameter* is introduced. In this section, the connection of these concepts to the previously introduced tensor series is presented.

The orientation tensors are defined as the sum of the tensor product of the particle orientations within a reference volume element

$$o_{\mu_1 \ldots \mu_l} = \sum_i n_{\mu_1} \ldots n_{\mu_l}. \quad (68)$$

The traceless version of these tensors is called alignment tensors or deviatoric part and these tensors appear in the series expansion of the ODF, Eq. (5). The difference is that in the case of isotropic distribution, the orientation tensor would be the identity tensor, while the alignment tensor would be the zero tensor (zero alignment).

It is further possible and common to define scalar order parameters, which are connected to the second-order alignment tensor. Based on the eigenvalues of the second-order alignment tensor it is often useful to introduce an orientational order parameter $S \in [-\frac{1}{2}, 1]$, which accounts for the amount of anisotropy. The case $S = 1$ corresponds to total alignment and $S = 0$ corresponds to isotropy; $S = -\frac{1}{2}$ describes a situation where all fibres are aligned in a plane perpendicular to the eigenvector of the first eigenvalue. In the following, it is assumed that the eigenvalues are sorted according to the amount $|\lambda_1| \geq |\lambda_2| \geq |\lambda_3|$. The order parameter S and eigenvalues λ_i are related as follows:

$$\frac{2}{3} S = \lambda_1, \quad (69)$$

$$-\frac{1}{3} S - b_S = \lambda_2, \quad (70)$$

$$-\frac{1}{3} S + b_S = \lambda_3, \quad (71)$$

where $b_S = \operatorname{sign}(S) b$ and the biaxiality $b \in \left[0, \frac{1}{3}|S|\right]$ of the distribution [24].

The range of the order parameter S can be calculated as follows [6]:
Define the order parameter tensor $\mathbf{S}$ as

$$S_{ij} \; := \; \frac{3}{2}A_{ij} \tag{72}$$

and let $\boldsymbol{d}^1$ be the normalized eigenvector with respect to the according-to-amount largest eigenvalue S, then the scalar order parameter and the tensor are related as follows:

$$d^1_\mu \underbrace{S_{\mu\nu} d^1_\nu}_{=Sd^1_\mu} \; = \; S \quad (d^1_\mu d^1_\mu = 1). \tag{73}$$

Now consider

$$d^1_\mu S_{\mu\nu} d^1_\nu \; = \; d^1_\mu d^1_\nu \frac{3}{2N} \sum_{i=1}^{N} \overline{n^{(i)}_\mu n^{(i)}_\nu}\,, \tag{74}$$

$$= \; d^1_\mu d^1_\nu \frac{3}{2N} \sum_{i=1}^{N} \left(n^{(i)}_\mu n^{(i)}_\nu - \frac{1}{3}\delta_{\mu\nu} \right), \tag{75}$$

$$= \; \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} d^1_\mu d^1_\nu \left(3 n^{(i)}_\mu n^{(i)}_\nu - \delta_{\mu\nu} \right), \tag{76}$$

and with $d^1_\mu n^{(i)}_\mu =: x$

$$d^1_\mu S_{\mu\nu} d^1_\nu \; = \; \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} \left(3x^2 - 1 \right), \tag{77}$$

$$= \; \left\langle \frac{1}{2}(3x^2 - 1) \right\rangle. \tag{78}$$

As both $\boldsymbol{d}^1$ and $\boldsymbol{n}^{(i)}$ are normalized, $d^1_\mu n^{(i)}_\mu \in [-1,1]$. From Eq. (78) follows that $S \in [-\frac{1}{2},1]$, and with the second Legendre polynomial $P_2(x) = 1/2(3x^2 - 1)$ one can rewrite the equation in the following ways:

$$S \; = \; \langle P_2(x) \rangle\,, \tag{79}$$

$$= \; \left\langle P_2(\boldsymbol{d}^1 \cdot \boldsymbol{n}) \right\rangle, \tag{80}$$

$$= \; \langle P_2(\cos\alpha) \rangle\,, \tag{81}$$

where α is the angle between $\boldsymbol{d}^1$ and $\boldsymbol{n}$.

The eigenvectors of the second-order alignment tensor are appropriate estimates for the directions of the main material symmetry axes derived from the orientation distribution function. The eigenvector of the (by absolute value) largest eigenvalue determines the symmetry axis of a transversely isotropic material or the main fibre orientation in an orthotropic material. For the transversely isotropic material one needs to distinguish two cases: if S is positive, the symmetry axis is the average direction of the fibres and, if S is negative, the fibres are mostly oriented in a plane perpendicular to the eigenvector.

6. PRACTICAL EXAMPLES FOR THE USE OF ORIENTATION TENSORS IN CONSTITUTIVE THEORY

6.1. Molecular gases

The use of symmetric irreducible tensors to represent a spherical function dates back to at least Ludwig Waldmann [1] in the theory of molecular gases.

6.2. The anisotropic dielectric tensor in uniaxial nematic liquid crystals

One example for the use of alignment tensors in constitutive equations is given in the book by Hess [21] for liquid crystals.

Considering the Maxwell equations for electromagnetic theory,

$$\nabla \cdot \boldsymbol{D} = \rho, \tag{82}$$

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}, \tag{83}$$

$$\nabla \cdot \boldsymbol{B} = 0, \tag{84}$$

$$\nabla \times \boldsymbol{H} = \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t}, \tag{85}$$

these are underdetermined. Constitutive equations are needed to determine the additional fields $\boldsymbol{D}$ and $\boldsymbol{H}$ in terms of $\boldsymbol{E}$ and $\boldsymbol{B}$. For the special case of linear isotropic and instantaneous materials

$$\boldsymbol{D} = \varepsilon \boldsymbol{E}, \tag{86}$$

$$\boldsymbol{H} = \frac{1}{\mu}\boldsymbol{B} \tag{87}$$

are used. For anisotropic materials, such as birefringent crystals, the scalar coefficients need to be changed to tensorial coefficients. Liquid crystals, although liquids, show birefringence, which gave rise to the name. The symmetric traceless part of the dielectric tensor is proportional to the [second-order] alignment tensor [21]:

$$\overset{\frown}{\boldsymbol{\varepsilon}} = \varepsilon_a \mathbf{a}. \tag{88}$$

Therefore, the constitutive equation for $\boldsymbol{D}$ reads

$$\boldsymbol{D} = \varepsilon_a \mathbf{a} \cdot \boldsymbol{E}. \tag{89}$$

The coefficient ε_a depends on the density of the material and on the difference $\alpha_{\parallel} - \alpha_{\perp}$ of the molecular polarizabilities parallel and perpendicular to $\boldsymbol{n}$.

6.3. Rheology of fibre suspensions

When elongated particles, e.g. granular media made of elongated particles, liquid crystals, or fibres suspended in a liquid flow, they change orientations in the presence of velocity gradients. The (mis)-alignment of the 'fibres' also introduces an additional viscosity [25]. Based on the orientation tensors one can define model 1 and model 2:

$$\mu_{p1} = \frac{\mu_p a_{1122}}{\mu}, \tag{90}$$

$$\mu_{p2} = \frac{\mu_p a_{11mn\dot{\gamma}_{nm}}}{2\mu\dot{\gamma}_{12}} \quad m,n = 1,2, \tag{91}$$

where $\dot{\gamma}$ is the airflow strain rate, $\dot{\gamma}_{nm} = \frac{\partial u_m}{\partial x_n} + \frac{\partial u_n}{\partial x_m}$; μ is the air dynamic viscosity; and μ_p is the additional viscosity of fibres.

6.4. Solid mechanics of anisotropic materials

In solids containing fibres, the mechanical properties can become anisotropic. Also in this case, the anisotropy can be described by using alignment or orientation tensors. For fibre concrete, this is discussed e.g. in [8,10,12]. The proposed constitutive equation for the dependence of the stresses on the deformation in the elastic range is given by

$$\begin{aligned}\mathbf{S}^{\mathrm{SFRC}}(\mathbf{E},\mathbf{A}) &= \nu_{\mathrm{m}}\,(\lambda\,\mathrm{tr}(\mathbf{E})\mathbf{I}+2\mu\mathbf{E}) \\ &\quad +\nu_{\mathrm{f}}\kappa_{\mathrm{fg}}\left(\alpha\,\mathrm{tr}(\mathbf{EA})\mathbf{A}^T+\beta\left((\mathbf{AE})^T+(\mathbf{EA})^T\right)\right). \end{aligned} \tag{92}$$

Another example is short fibre reinforced plastics [15]. Here the orientation averaging of a transversely isotropic material leads to orientation tensors in the equation for the anisotropic short fibre material.

7. CONCLUSION

This paper gives an overview how spherical harmonical functions can be represented by the use of symmetric traceless tensors. Starting from a representation of a function on a unit sphere in terms of a basis formed by spherical harmonics, it is then shown that spherical harmonics can be represented by symmetric traceless tensors. Further, examples for the use of alignment or orientation tensors in constitutive theory are presented.

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APPENDIX A

DEFINITIONS

Definition 4 (Tensor product [18])**.** *Assume* $\mathbf{A}$ *is a tensor of the order m and* $\mathbf{B}$ *is a tensor of the order n, with components* $a_{\mu_1\ldots\mu_m}$ *and* $b_{\nu_1\ldots\nu_n}$ *in three dimensions. Then the* 3^{m+n} *scalars*

$$c_{\mu_1\ldots\mu_m\nu_1\ldots\nu_n} \quad = \quad a_{\mu_1\ldots\mu_m}b_{\nu_1\ldots\nu_n} \tag{93}$$

give the components of the tensor $\mathbf{C}$ *of the order* $m+n$*. We denote it by* $\mathbf{C}=\mathbf{AB}$ *and we call it the tensor product of* $\mathbf{A}$ *and* $\mathbf{B}$.

Definition 5 (Dyadic product)**.** *The product of two tensors of the order 1 in three dimensions* $a=(a_1,a_2,a_3)$ *and* $b=(b_1,b_2,b_3)$ *gives a tensor of the order 2 with the elements*

$$c_{ij} \quad = \quad a_ib_j \quad (i,j=1,2,3), \tag{94}$$

i.e. the tensor product results in the matrix

$$\begin{pmatrix} a_1b_1 & a_1b_2 & a_1b_3 \\ a_2b_1 & a_2b_2 & a_2b_3 \\ a_3b_1 & a_3b_2 & a_3b_3 \end{pmatrix}. \tag{95}$$

Definition 6 (Vector space). *A vector space over a field F is a set V together with two binary operations that satisfy the following eight axioms:*
- *associativity of addition: $u+(v+w)=(u+v)+w$;*
- *commutativity of addition: $u+v=v+u$;*
- *(identity element of addition) there exists an element $0 \in V$ called the* zero element, *such that $v+0=v$ for all $v \in V$;*
- *(inverse element of addition) for every $v \in V$ there exists an element $-v \in V$, called the* additive inverse *of v, such that $v+(-v)=0$;*
- *distributivity of scalar multiplication with respect to vector addition: $a(u+v)=au+av$;*
- *distributivity of scalar multiplication with respect to field addition: $(a+b)v=av+bv$;*
- *compatibility of scalar multiplication with field multiplication: $a(bv)=(ab)v$;*
- *identity element of scalar multiplication: $1v=v$, where 1 is the multiplicative identity in F.*

Definition 7 (Scalar product). *A* scalar product *or* inner product *on a real vector space V is a positive definite symmetric bilinear form $\langle\cdot,\cdot\rangle : V\times V \to \mathbb{R}$, which means for $x,y,z \in V$ and $\lambda \in \mathbb{R}$, the following requirements are fulfilled:*
- *bilinear:*
  $\langle x+y,z\rangle = \langle x,z\rangle + \langle y,z\rangle$
  $\langle x,y+z\rangle = \langle x,z\rangle + \langle y,z\rangle$
  $\langle x,\lambda y\rangle = \lambda\langle x,z\rangle$
- *symmetric: $\langle x,y\rangle = \langle y,x\rangle$*
- *positive definite: $\langle x,x\rangle \geq 0$, and $\langle x,x\rangle = 0$ if and only if $x=0$.*

Definition 8 (Norm). *A* norm *on a real vector space V is a function $\|\cdot\| : V \to [0,\infty)$ that fulfils for all $x,y \in V, \alpha \in \mathbb{R}$:*
- *definiteness: $\|x\|=0 \Leftrightarrow x=0$ (or $\|x\|=0 \Rightarrow x=0$?)*
- *homogenity: $\|\alpha x\| = |\alpha|\cdot\|x\|$*
- *triangle inequality: $\|x+y\| \leq \|x\|+\|y\|$.*

APPENDIX B

TENSORS AS SPHERICAL HARMONICS

For every $\boldsymbol{n} \in S^2$ exist angles $\varphi \in [0,2\pi), \vartheta \in [0,\pi)$ such that

$$\boldsymbol{n} = (n_1,n_2,n_3) = (\cos\varphi\sin\vartheta, \sin\varphi\sin\vartheta, \cos\vartheta). \tag{96}$$

With Eq. (96) we can express the spherical harmonics in cartesian coordinates

$$Y_0^0(\vartheta,\varphi) = \frac{1}{4\pi} = Y_0^0(n_1,n_2,n_3), \tag{97}$$

$$Y_1^{-1}(\vartheta,\varphi) = \frac{3}{4\pi}\sin\varphi\sin\vartheta = \frac{3}{4\pi}n_2 = Y_1^{-1}(n_1,n_2,n_3), \tag{98}$$

$$Y_1^0(\vartheta,\varphi) = \frac{3}{4\pi}\cos\vartheta = \frac{3}{4\pi}n_3 = Y_1^0(n_1,n_2,n_3), \tag{99}$$

$$Y_1^1(\vartheta,\varphi) = \frac{3}{4\pi}\cos\varphi\sin\vartheta = \frac{3}{4\pi}n_1 = Y_1^1(n_1,n_2,n_3), \tag{100}$$

and with

$$\sin(2\varphi) = 2\sin\varphi\cos\varphi, \tag{101}$$

$$\cos(2\varphi) = \cos^2\varphi - \sin^2\varphi \tag{102}$$

follows

$$
\begin{aligned}
Y_2^{-2}(\vartheta,\varphi) &= \sqrt{\frac{45}{28\pi}}\sin^2\vartheta\sin(2\varphi) \overset{(101)}{=} 2\sqrt{\frac{45}{28\pi}}\cos\varphi\sin\vartheta\sin\varphi\sin\vartheta \\
&= 2\sqrt{\frac{45}{28\pi}}n_1n_2 = Y_2^{-2}(n_1,n_2,n_3), && (103)\\
Y_2^{-1}(\vartheta,\varphi) &= -\sqrt{\frac{15}{4\pi}}\sin\vartheta\cos\vartheta\sin\varphi = -\sqrt{\frac{15}{4\pi}}n_2n_3 = Y_2^{-1}(n_1,n_2,n_3), && (104)\\
Y_2^{0}(\vartheta,\varphi) &= \sqrt{\frac{5}{128\pi}}(3\cos^2\vartheta-1) = 3\sqrt{\frac{5}{128\pi}}n_3^2 - \sqrt{\frac{5}{128\pi}}(n_1^2+n_2^2+n_3^2) = Y_2^0(n_1,n_2,n_3), && (105)\\
Y_2^{1}(\vartheta,\varphi) &= -\sqrt{\frac{15}{4\pi}}\sin\vartheta\cos\vartheta\cos\varphi = -\sqrt{\frac{15}{4\pi}}n_1n_3 = Y_2^{1}(n_1,n_2,n_3), && (106)\\
Y_2^{2}(\vartheta,\varphi) &= \sqrt{\frac{45}{28\pi}}\sin^2\vartheta\cos(2\varphi) \overset{(102)}{=} \sqrt{\frac{45}{28\pi}}(\sin^2\vartheta\cos^2\varphi - \sin^2\vartheta\sin^2\varphi)\\
&= \sqrt{\frac{45}{28\pi}}(n_1^2-n_2^2) = Y_2^2(n_1,n_2,n_3). && (107)
\end{aligned}
$$

The symmetric traceless tensors that correspond to the spherical harmonics are then given by (with respect to the canonical basis)

$$
[a^{0,0}] = \frac{1}{4\pi}, \qquad [a^{1,-1}] = \begin{pmatrix} 0 \\ \sqrt{\frac{3}{4\pi}} \\ 0 \end{pmatrix}, \qquad [a^{1,0}] = \begin{pmatrix} 0 \\ 0 \\ \sqrt{\frac{3}{4\pi}} \end{pmatrix}, \qquad [a^{1,1}] = \begin{pmatrix} \sqrt{\frac{3}{4\pi}} \\ 0 \\ 0 \end{pmatrix} \tag{108}
$$

and

$$
\begin{aligned}
[a^{2,-2}] &= \begin{pmatrix} 0 & \sqrt{\frac{45}{28\pi}} & 0 \\ \sqrt{\frac{45}{28\pi}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, && (109)\\
\left[a^{2,-1}\right] &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2}\sqrt{\frac{15}{4\pi}} \\ 0 & -\frac{1}{2}\sqrt{\frac{15}{4\pi}} & 0 \end{pmatrix}, && (110)\\
\left[a^{2,0}\right] &= \begin{pmatrix} -\sqrt{\frac{5}{128\pi}} & 0 & 0 \\ 0 & -\sqrt{\frac{5}{128\pi}} & 0 \\ 0 & 0 & 2\sqrt{\frac{5}{128\pi}} \end{pmatrix}, && (111)\\
\left[a^{2,1}\right] &= \begin{pmatrix} 0 & 0 & -\frac{1}{2}\sqrt{\frac{15}{4\pi}} \\ 0 & 0 & 0 \\ -\frac{1}{2}\sqrt{\frac{15}{4\pi}} & 0 & 0 \end{pmatrix}, && (112)\\
\left[a^{2,2}\right] &= \begin{pmatrix} \sqrt{\frac{45}{28\pi}} & 0 & 0 \\ 0 & -\sqrt{\frac{45}{28\pi}} & 0 \\ 0 & 0 & 0 \end{pmatrix}. && (113)
\end{aligned}
$$

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Sfäärilise funktsiooni tensorrea kasutamine orienteeritud osakesi sisaldava materjali olekuvõrrandi teoorias

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On esitatud didaktiline sissejuhatus sfäärilise funktsiooni tensorreaksarendusse, et seda kasutada orienteeritud osakesi sisaldava materjali olekuvõrrandi teoorias. Funktsiooni, mille argumendiks on kaks nurka, näiteks orientatsiooni jaotustihedusfunktsioon, arendatakse mitmetes rakendustes ritta sümmeetrilistest mitteredutseeruvatest tensoritest. Artiklis on selgitatud sellist reaksarendust, alustades ülevaatega funktsioonist, mis on defineeritud ühiksfääril sfääriliste harmoonikute kui ühe võimaliku baasi kaudu. Seejärel on selgitatud seost sfääriliste harmoonikute ja selliste sümmeetriliste tensorite vahel, mille jälg võrdub nulliga. See moodustab aluse, et mõista orientatsiooni- ja joonduvustensoreid kui ka nende seost orientatsiooni jaotusfunktsiooniga. Materjali esituslaad on didaktilise kallakuga ja erineb mujal leiduvast teoreem-tõestus-esitusviisist, kus koheselt alustatakse sümmeetriliste tensoritega.