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# Invariant formulation of hyperelastic transverse isotropy based on polyconvex free energy functions

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**Abstract**

In this paper we propose a formulation of polyconvex anisotropic hyperelasticity at finite strains. The main goal is the representation of the governing constitutive equations within the framework of the invariant theory which automatically fulfill the polyconvexity condition in the sense of Ball in order to guarantee the existence of minimizers. Based on the introduction of additional argument tensors, the so-called structural tensors, the free energies and the anisotropic stress response functions are represented by scalar-valued and tensor-valued isotropic tensor functions, respectively. In order to obtain various free energies to model specific problems which permit the matching of data stemming from experiments, we assume an additive structure. A variety of isotropic and anisotropic functions for transversely isotropic material behaviour are derived, where each individual term fulfills a priori the polyconvexity condition. The tensor generators for the stresses and moduli are evaluated in detail and some representative numerical examples are presented. Furthermore, we propose an extension to orthotropic symmetry.


*Keywords:* Non-linear elasticity; Anisotropy; Polyconvexity; Existence of minimizers

## 1. Introduction

Anisotropic materials have a wide range of applications, e.g. in composite materials, in crystals as well as in biological–mechanical systems. The study of these different materials involves many topics, including manufacturing processes, anisotropic elasticity and anisotropic inelasticity, and micro-mechanics see e.g. Jones (1975). In this paper we will focus on a phenomenological description of anisotropic elasticity at large strains, for small strain formulations see e.g. Ting (1996). The main goal of this work is the construction of polyconvex anisotropic free energy functions, particularly for transverse isotropic materials. Proposed transversely isotropic free energy functions in the literature are often based on a direct extension of the small strain theory to the case of finite deformations by replacing the linear strain tensor with the

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Green–Lagrange strain tensor see e.g. Spencer (1987b). Weiss et al. (1996) presented a model for applications to biological soft tissues for fully incompressible material behaviour. They introduced an exponential function in terms of the so-called mixed invariants. In the recent work of Holzapfel et al. (2000) a new constitutive orthotropic model for the simulation of arterial walls has been proposed, where each layer of the artery is modeled as a fiber-reinforced material. In the proposed model the terms in the mixed invariants, with respect to several preferred directions, are additively decoupled. That means the model can be considered as the superposition of different transverse isotropic models. For an overview and a comparative study of several mechanical models in biomechanical systems see also Holzapfel et al. (2000). A model for nearly incompressible, transversely isotropic materials for the description of reinforced rubber-like materials is given in Rüter and Stein (2000); they also developed an error estimator for the measurement of the discretization error within the finite element concept. Anisotropic models for the simulation of anisotropic shells have been proposed by Lürding (2001) and Itskov (2001). A general framework for representation of anisotropic elastic materials by symmetric irreducible tensors based on series expansions of elastic free energy functions in terms of harmonic polynomials was proposed by Hackl (1999). The advantage of this approach is its ability to derive effective schemes of parameter identifications. A set of physically motivated deformation invariants for materials exhibiting transverse isotropic behaviour was developed by Criscione et al. (2001). The authors suggest that this approach is potentially useful for solving inverse problems due to several orthogonality conditions.

In contrast to this, no analysis of general convexity conditions for anisotropic materials, such as polyconvexity, has been proposed in the literature to the knowledge of the authors. We will focus on the case of transverse isotropy at finite strains which automatically satisfy the so-called polyconvexity condition within the framework of the invariant theory. The complex mechanical behaviour of elastic materials at large strains with an oriented internal structure can be described with tensor-valued functions in terms of several tensor variables, the deformation gradient and additional structural tensors. General invariant forms of the constitutive equations lead to rational strategies for the modelling of the complex anisotropic response functions. Based on representation theorems for tensor functions the general forms can be derived and the type and minimal number of the scalar variables entering the constitutive equations can be given. For an introduction to the invariant formulation of anisotropic constitutive equations based on the concept of structural tensors, also denoted as the concept of integrity bases, and their representations as isotropic tensor functions see Spencer (1971), Boehler (1979, 1987), Betten (1987) and Schröder (1996). In this context see also Smith and Rivlin (1957, 1958).

The main goal of this paper is the establishment of invariant forms of the stress response function $\widehat{\boldsymbol{S}}(\bullet)$ which are derived from a scalar-valued free energy function $\hat{\psi}(\bullet)$. These invariant forms automatically satisfy the symmetry relations of the considered body. Furthermore, they are automatically invariant under coordinate transformations of elements of the material symmetry group. Thus the values of the free energy function and the values of the stresses can be considered as invariants under all transformations of the elements of the material symmetry group. For the representation of the scalar-valued and tensor-valued functions the set of scalar invariants, the integrity bases and the generating set of tensors are required. For detailed representations of scalar- and tensor-valued functions we refer to Wang (1969a,b, 1970, 1971), Smith et al. (1963), Smith (1965, 1970, 1971), and Zheng and Spencer (1993a,b). The integrity bases for polynomial isotropic scalar-valued functions are given by Smith (1965) and the generating sets for the tensor functions are derived by Spencer (1971). For the classification of material and physical symmetries see Zheng and Boehler (1994).

The mathematical treatment of boundary value problems is mainly based on the direct methods of variations, i.e. finding a minimizing deformation of the elastic free energy subject to the specific boundary conditions. Existence of minimizers of some variational principles in finite elasticity is based on the concept of quasiconvexity, introduced by Morrey (1952), which ensures that the functional to be minimized is weakly lower semi-continuous. This inequality condition is rather complicated to handle since it is an integral inequality. Thus, a more important concept for practical use is the notion of polyconvexity in the sense of Ball (1977a,b) (in this context see also Marsden and Hughes, 1983 and Ciarlet, 1988). For isotropic material response functions there exist some models, e.g. the Ogden-, Mooney-Rivlin- and Neo-Hooke-type models, which satisfy this concept. Furthermore, for isochoric–volumetric decouplings some forms of polyconvex energies have been proposed by Dacorogna (1989). Some simple stored energy functions, e.g. of St. Venant–Kirchhoff-type or formulations based on the so-called Hencky tensor, are however not polyconvex (see Ciarlet, 1988, Raoult, 1986 and Neff, 2000). It can be shown that polyconvexity of the stored energy implies that the corresponding acoustic tensor is elliptic for all deformations. The precise difference between the local property of ellipticity and the non-local condition of quasiconvexity is still an active field of research. Polyconvexity does not conflict with the possible non-uniqueness of equilibrium solutions, since it guarantees only the existence of at least one minimizing deformation. It is possible that several metastable states and several absolute minimizers exist, though even so one might conjecture that apart from trivial symmetries the absolute minimizer is unique, at least for the pure Dirichlet boundary value problem. We remark, following Ball (1977a,b), that polyconvexity implies unqualified existence for all boundary conditions and body forces, which might be somewhat unrealistic. The proof that some energy is elliptic for some reasonable range of deformation gradients is in general not enough to establish an existence theorem.

This paper is organized as follows. In Section 2 we present the fundamental kinematic relations at finite strains and the reduced forms which automatically fulfill the objectivity condition. After that we focus on the continuum mechanical modelling of anisotropic elasticity based on the concept of structural tensors. Section 3 is concerned with the construction of transversely isotropic material response. The integrity basis is given and special model problems are discussed. One part of this section deals with isotropic free energy terms, where some well-known, as well as some new functions are discussed in detail. The main part of this section is concerned with polyconvex transversely isotropic functions. For all proposed ansatz functions the polyconvexity condition is proved. Furthermore, we give geometrical interpretations of some of the polyconvex polynomial invariants. The representation for the stresses and moduli is given in detail for the Lagrangian description as well as the expression for the Kirchhoff stresses. The problem of the stress-free reference configuration and the linearized behaviour near the natural state is discussed in Section 4. Here we identify the expressions of the material parameters involved in the invariant formulation with the parameters of the classical formulation for the linearized quantities. An extension to orthotropic material response is proposed in Section 5 and a short summary of the variational and finite element formulation and the consistent linearization is given in Section 6. The following section presents two numerical examples: the three dimensional analysis of a tapered cantilever and the two dimensional simulation of the elongation of a perforated plate. In the extensive appendix we have summarized the lengthy proofs of the polyconvexity of the individual terms.

## 2. Continuum mechanics: foundations

In the following we consider hyperelastic materials which postulate the existence of a so-called Helmholtz free–energy function $\psi$. The constitutive equations have to fulfill several requirements: the *concept of material symmetry* and the *principle of material frame indifference*, also denoted as *principle of material objectivity*. Thus, the constitutive functions for anisotropic solids must satisfy the combined material frame indifference and the material symmetry condition, which requires them to be an isotropic tensor function. After giving some fundamental kinematic relations and presenting the well-known reduced forms for the constitutive equations which automatically fulfill the objectivity condition we focus on the continuum mechanical modelling of anisotropic elasticity within the framework of isotropic tensor functions based on the concept of structural tensors.

### 2.1. Notation

For $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^3$ we let $\langle \boldsymbol{a}, \boldsymbol{b} \rangle_{\mathbb{R}^3}$ denote the scalar product on $\mathbb{R}^3$ with norm $\|\boldsymbol{a}\|_{\mathbb{R}^3} = \langle \boldsymbol{a}, \boldsymbol{a} \rangle_{\mathbb{R}^3}^{1/2}$. We denote with $\mathbb{M}^{3\times3}$ the set of real $3 \times 3$ matrices and by skew $(\mathbb{M}^{3\times3})$ the skew-symmetric real $3 \times 3$ matrices. The standard Euclidean scalar product on $\mathbb{M}^{3\times3}$ is given by $\langle \boldsymbol{H}, \boldsymbol{B} \rangle_{\mathbb{M}^{3\times3}} = \mathrm{tr}[\boldsymbol{H}\boldsymbol{B}^{\mathrm{T}}]$ and subsequently we have $\|\boldsymbol{H}\|^2_{\mathbb{M}^{3\times3}} = \langle \boldsymbol{H}, \boldsymbol{H} \rangle_{\mathbb{M}^{3\times3}}$. $P\mathbb{S}\mathrm{ym}$ characterizes the set of positive definite symmetric $\mathbb{M}^{3\times3}$ matrices. With $\mathrm{Adj}\,\boldsymbol{H}$ we denote the adjugate matrix of transposed cofactors $\mathrm{Cof}(\boldsymbol{H})$ such that $\mathrm{Adj}\,\boldsymbol{H} = \det[\boldsymbol{H}]\boldsymbol{H}^{-1} = \mathrm{Cof}(\boldsymbol{H})^{\mathrm{T}}$ if $\boldsymbol{H} \in GL(3, \mathbb{R})$, where $GL(3, \mathbb{R})$ characterizes the set of all invertible $3 \times 3$-tensors. The identity matrix on $\mathbb{M}^{3\times3}$ will be denoted by $\mathbb{1}$ or $\mathbf{1}$, so that $\mathrm{tr}[\boldsymbol{H}] = \langle \boldsymbol{H}, \mathbb{1} \rangle = \boldsymbol{H} : \mathbf{1}$. The index notation of $\boldsymbol{A} : \boldsymbol{H}$ is e.g. $A_{AB}H^{AB}$ and that of $\boldsymbol{H}\boldsymbol{a} = \boldsymbol{H} \cdot \boldsymbol{a}$ is e.g. $H_{AB}a^B$. In the following we skip the index $\mathbb{R}^3$, $\mathbb{M}^{3\times3}$ where there is no danger of confusion. Furthermore, $\partial_F W(\boldsymbol{F})$, $\partial_C W(\boldsymbol{C})$, $D_C W$ and $\partial_F W(\boldsymbol{F}).\boldsymbol{H}$, $\partial_F^2 W(\boldsymbol{F}).(\boldsymbol{H}, \boldsymbol{H})$ denote Frechet derivatives (in this context see Appendix A, Lemma A.13).

### 2.2. Geometry and kinematics

The body of interest in the reference configuration is denoted with $\mathscr{B} \subset \mathbb{R}^3$, parametrized in $\boldsymbol{X}$ and the current configuration with $\mathscr{S} \subset \mathbb{R}^3$, parametrized in $\boldsymbol{x}$. The non-linear deformation map $\boldsymbol{\varphi}_t : \mathscr{B} \to \mathscr{S}$ at time $t \in \mathbb{R}_+$ maps points $\boldsymbol{X} \in \mathscr{B}$ onto points $\boldsymbol{x} \in \mathscr{S}$. The deformation gradient $\boldsymbol{F}$ is defined by

$$\boldsymbol{F}(\boldsymbol{X}) := \nabla \boldsymbol{\varphi}_t(\boldsymbol{X}) \tag{2.1}$$

with the Jacobian $J(\boldsymbol{X}) := \det \boldsymbol{F}(\boldsymbol{X}) > 0$. The index notation of $\boldsymbol{F}$ is $F^a_A := \partial x^a / \partial X^A$. An important strain measure, the right Cauchy–Green tensor, is defined by

$$\boldsymbol{C} := \boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} \quad \text{with } C_{AB} = F^a_A F^b_B g_{ab}, \tag{2.2}$$

where $\boldsymbol{g}$ denotes the covariant metric tensor in the current configuration. The standard covariant metric tensors $\boldsymbol{G}$ and $\boldsymbol{g}$ within the Lagrange and Eulerian settings appear in the index representation $G_{AB}$ and $g_{ab}$, respectively. Thus the contravariant metric tensors $\boldsymbol{G}^{-1}$ and $\boldsymbol{g}^{-1}$ have the index representation $G^{AB}$ and $g^{ab}$, respectively. For the representations in Cartesian coordinates we arrive at the simple expressions $G_{AB} = G^{AB} = \delta_{AB}$ for Lagrangian metric tensors and $g_{ab} = g^{ab} = \delta_{ab}$ for the Eulerian metric tensors. For the geometrical interpretations of the polynomial invariants in the following sections we often use expressions based on the mappings of the area and volume elements. Let $\boldsymbol{N}\,\mathrm{d}A$ and $\boldsymbol{n}\,\mathrm{d}a$ denote the infinitesimal area vectors and $\mathrm{d}V$ and $\mathrm{d}v$ denote the infinitesimal volume elements defined in the reference and the current configuration, respectively, then

$$\boldsymbol{n}\,\mathrm{d}a = \mathrm{Cof}[\boldsymbol{F}]\boldsymbol{N}\,\mathrm{d}A \quad \text{and} \quad \mathrm{d}v = \det[\boldsymbol{F}]\,\mathrm{d}V \tag{2.3}$$

holds. The first part of Eq. (2.3) is the well-known Nanson's formula. It should be mentioned that the argument $(\boldsymbol{F}, \mathrm{Adj}\,\boldsymbol{F}, \det \boldsymbol{F})$, with $\mathrm{Adj}\,\boldsymbol{F} = (\mathrm{Cof}\,\boldsymbol{F})^{\mathrm{T}}$, plays an important role in the definition of polyconvexity; this will be discussed in detail in Section 3.

### 2.3. Hyperelasticity and invariance conditions

We consider hyperelastic materials which postulate the existence of a so-called Helmholtz free-energy function $\psi$, assumed to be defined per unit reference volume. Here we focus on the dependence of $\psi$ solely in the deformation gradient, i.e. $\psi = \hat{\psi}(\boldsymbol{F}, \bullet)$. The argument $(\bullet)$ in the free energy function denotes additional tensor arguments, which characterize the anisotropy of the material; they will be discussed in the following sections. We consider perfect elastic materials, which means that the internal dissipation $\mathscr{D}_{\mathrm{int}}$ is zero for every admissible process. The constitutive equations for the stresses are obtained by evaluation of the Clausius–Planck inequality, neglecting thermal effects, in the form

$$\mathscr{D}_{\text{int}} = \boldsymbol{P} : \dot{\boldsymbol{F}} - \dot{\psi} = (\boldsymbol{P} - \partial_F \psi) : \dot{\boldsymbol{F}} \geqslant 0 \rightarrow \boldsymbol{P} = \partial_F \psi. \tag{2.4}$$

$\boldsymbol{P}$ characterizes the first Piola–Kirchhoff stress tensor and $\dot{\boldsymbol{F}}$ denotes the material time derivative of the deformation gradient, which is identical to the material velocity gradient. Furthermore, $\partial_F(\bullet)$ is the abbreviation for $\partial(\bullet)/\partial\boldsymbol{F}$.

The principle of material frame indifference requires the invariance of the constitutive equation under superimposed rigid body motions onto the current configuration, i.e. under the mapping $\boldsymbol{x} \rightarrow \boldsymbol{Q}\boldsymbol{x}$ the condition $\psi(\boldsymbol{F}) = \psi(\boldsymbol{Q}\boldsymbol{F})$ holds $\forall \boldsymbol{Q} \in \mathrm{SO}(3)$. For the stress response this principle leads with (2.4 second part) to the invariance relations

$$\boldsymbol{S}(\boldsymbol{F}) = \boldsymbol{S}(\boldsymbol{Q}\boldsymbol{F}), \quad \boldsymbol{Q}\boldsymbol{P}(\boldsymbol{F}) = \boldsymbol{P}(\boldsymbol{Q}\boldsymbol{F}), \quad \boldsymbol{Q}\boldsymbol{\sigma}(\boldsymbol{F})\boldsymbol{Q}^{\mathrm{T}} = \boldsymbol{\sigma}(\boldsymbol{Q}\boldsymbol{F}) \qquad \forall \boldsymbol{Q} \in \mathrm{SO}(3). \tag{2.5}$$

Reduced constitutive equations which fulfill a priori the principle of material objectivity (2.5) yield e.g. the functional dependence $\psi = \hat{\psi}(\boldsymbol{C}) = \hat{\psi}(\boldsymbol{C}(\boldsymbol{F}, \boldsymbol{g}))$ (see e.g. Truesdell and Noll, 1965). If we assume the free energy function to be a function of the right Cauchy–Green tensor $\hat{\psi}(\boldsymbol{C})$ or of the spatial metric $\boldsymbol{g}$ we obtain with the chain rule the expressions

$$\boldsymbol{S} = 2\partial_C \hat{\psi}(\boldsymbol{C}) \quad \text{and} \quad \boldsymbol{\tau} = J\boldsymbol{\sigma} = 2\partial_g \hat{\psi}(\boldsymbol{C}(\boldsymbol{F}, \boldsymbol{g})) \tag{2.6}$$

(see e.g. Marsden and Hughes, 1983). The Eq. $(2.6)_2$ is the so-called Doyle-Ericksen formula. $\boldsymbol{S}$, $\boldsymbol{\tau}$ and $\boldsymbol{\sigma}$ denote the Second Piola–Kirchhoff stresses, the Kirchhoff stresses and the Cauchy stresses, respectively.

In the case of anisotropy we introduce a material symmetry group $\mathscr{G}_k$ with respect to a local reference configuration, which characterizes the anisotropy class of the material. The elements of $\mathscr{G}_k$ are denoted by the unimodular tensors ${}^i\boldsymbol{Q} | i = 1, \ldots, n$. The concept of material symmetry requires that the response be invariant under transformations with elements of the symmetry group, i.e.

$$\hat{\psi}(\boldsymbol{F}\boldsymbol{Q}) = \hat{\psi}(\boldsymbol{F}) \quad \forall \boldsymbol{Q} \in \mathscr{G}_k, \boldsymbol{F}. \tag{2.7}$$

Thus superimposed rotations and reflections on the reference configuration with elements of the material symmetry group do not influence the behaviour of the anisotropic material. Equivalently, we can write condition (2.7) in terms of the stress response function

$$\boldsymbol{P}(\boldsymbol{F}\boldsymbol{Q}) = \boldsymbol{P}(\boldsymbol{F})\boldsymbol{Q} \quad \forall \boldsymbol{Q} \in \mathscr{G}_k, \boldsymbol{F}. \tag{2.8}$$

We say that the function $\psi$ in (2.7) or $\boldsymbol{P}$ in the latter equation are $\mathscr{G}_k$-invariant functions. Without any restrictions we set $\mathscr{G}_k \subset \mathrm{SO}(3)$, where SO(3) characterizes the special orthogonal group. Based on the mapping $\boldsymbol{X} \rightarrow \boldsymbol{Q}^{\mathrm{T}}\boldsymbol{X}$ for arbitrary rotation tensors $\boldsymbol{Q} \in \mathrm{SO}(3)$ we get from the requirement of an isotropic tensor function $\boldsymbol{\sigma}(\boldsymbol{F}) = \boldsymbol{\sigma}(\boldsymbol{F}\boldsymbol{Q})$ $\forall \boldsymbol{Q} \in \mathrm{SO}(3)$ the relations

$$\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{S}(\boldsymbol{F})\boldsymbol{Q} = \boldsymbol{S}(\boldsymbol{F}\boldsymbol{Q}), \quad \boldsymbol{P}(\boldsymbol{F})\boldsymbol{Q} = \boldsymbol{P}(\boldsymbol{F}\boldsymbol{Q}) \qquad \forall \boldsymbol{Q} \in \mathrm{SO}(3). \tag{2.9}$$

Thus it is clear that material symmetries impose several restrictions on the form of the constitutive functions of the anisotropic material. In order to work out the explicit restrictions for the individual symmetry groups, or more reasonably to point out general forms of the functions which fulfill these restrictions, it is necessary to use representation theorems for anisotropic tensor functions. To sum up, the constitutive expressions must satisfy the combined material frame indifference and the material symmetry condition, which requires them to be isotropic tensor functions with respect to an extended tensorial argument list. This topic is discussed in the following section.

### 2.4. Isotropic tensor functions for anisotropic material response

In this section we point out the main ingredients for deriving isotropic tensor functions for anisotropic solids. The main idea is the extension of $\mathscr{G}_k$-invariant functions into functions which are invariant under a

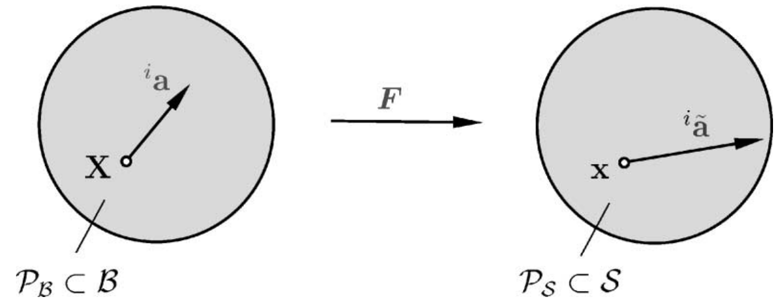


Fig. 1. Preferred directions ${}^i\boldsymbol{a}$ and ${}^i\tilde{\boldsymbol{a}}$ in the neighborhoods $\mathscr{P}_\mathscr{B} \subset \mathscr{B}$ and $\mathscr{P}_\mathscr{S} \subset \mathscr{S}$ of the points $\mathbf{X} \in \mathscr{B}$ and $\boldsymbol{x} \in \mathscr{S}$, respectively.

larger group, here the special orthogonal group. This implies that it is in principle possible to transform an anisotropic constitutive function into an isotropic function through some tensors, the so-called structural tensors, which reflect the symmetry group of the considered material. The concept of structural tensors was first introduced in an attractive way with important applications by Boehler in 1978/1979, although some similar ideas might have been touched on earlier. For a brief overview of representation of tensor functions see Rychlewski and Zhang (1991). The symmetry group of a material is defined by (2.7) and (2.8). Here we only consider anisotropic materials which can be characterized by certain directions, lines or planes. That means that the anisotropy can be described by some unit vectors ${}^i\boldsymbol{a}$ and some second order tensors ${}^i\boldsymbol{M}$ defined in the reference configuration, in this context we refer to Zheng and Boehler (1994). Fig. 1 illustrates the preferred directions ${}^i\boldsymbol{a}$ and ${}^i\tilde{\boldsymbol{a}} := \boldsymbol{F}{}^i\boldsymbol{a}$ with respect to the reference and current configuration, respectively. In the following, we restrict ourselves to the cases of transverse isotropy and orthotropy, where the material symmetry can be characterized by a set of structural tensors of second order. Let $\mathscr{G}_M$ be the invariance group of the structural tensors, i.e.

$$\mathscr{G}_M := \{\boldsymbol{Q} \in \mathrm{SO}(3), \boldsymbol{Q} * \boldsymbol{\xi} = \boldsymbol{\xi}\}, \tag{2.10}$$

with $\boldsymbol{\xi} := \{{}^i\boldsymbol{M}\}$ and $i = 1$ for transversely isotropic, and $i = 1, 2(, 3)$ for orthotropic, materials. The transformations ${}^i\boldsymbol{Q}|i = 1, \ldots, n$ represent rotations and reflections with respect to preferred directions and planes. In the following, we skip the index ${}^i(\bullet)$ if there is no danger of confusion. The last term in (2.10) characterizes the mapping $\boldsymbol{\xi} \to \boldsymbol{Q} * \boldsymbol{\xi} := \{\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{Q}\}$. If $\mathscr{G}_M \equiv \mathscr{G}_K$, where $\mathscr{G}_K$ is defined by (2.7) and (2.8), then the invariance group preserves the characteristics of the anisotropic solid.

Let us assume the existence of a set of $\mathscr{G}_k$-invariant structural tensors $\boldsymbol{\xi}$. Then we can transform (2.7) into a function which is invariant under the special orthogonal group. This leads to a scalar-valued isotropic tensor function in an extended argument list. That means that rotations superimposed onto the reference configuration with the mappings $\boldsymbol{X} \to \boldsymbol{Q}^{\mathrm{T}}\boldsymbol{X}$ and $\boldsymbol{\xi} \to \boldsymbol{Q} * \boldsymbol{\xi}$ lead to the condition $\psi = \hat{\psi}(\boldsymbol{F}, \boldsymbol{\xi}) = \hat{\psi}(\boldsymbol{F}\boldsymbol{Q}, \boldsymbol{Q} * \boldsymbol{\xi})\ \forall \boldsymbol{Q} \in \mathrm{SO}(3)$. Due to the concept of material frame indifference we arrive at a further reduction of the constitutive equation of the form

$$\psi = \hat{\psi}(\boldsymbol{C}, \boldsymbol{\xi}) = \hat{\psi}(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{Q}, \boldsymbol{Q} * \boldsymbol{\xi}) \quad \forall \boldsymbol{Q} \in \mathrm{SO}(3), \tag{2.11}$$

which is the definition of an isotropic scalar-valued tensor function in the arguments $(\boldsymbol{C}, \boldsymbol{\xi})$. For the stresses we obtain the isotropic tensor-valued tensor function

$$\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{S}(\boldsymbol{C}, \boldsymbol{\xi})\boldsymbol{Q} = \boldsymbol{S}(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{Q}, \boldsymbol{Q} * \boldsymbol{\xi}) \quad \forall \boldsymbol{Q} \in \mathrm{SO}(3). \tag{2.12}$$

It should be noted that the function is anisotropic with respect to $\boldsymbol{C}$. Furthermore, the relation $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{S}(\boldsymbol{C}, \boldsymbol{\xi})\boldsymbol{Q} = \boldsymbol{S}(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{Q}, \boldsymbol{\xi})$ holds for transformations $\boldsymbol{Q} \in \mathscr{G}_k$ and only for these transformations, thus the set of structural tensors $\boldsymbol{M}$ characterizes the material symmetry as pointed out above. It should be noted that if $\mathscr{G}_k = \mathrm{SO}(3)$ the material is isotropic. There are further material symmetries which are finite subgroups of SO(3), for the different crystal classes (see e.g. Smith et al., 1963, Spencer, 1971 and the references therein).

## 3. Free energy function for transverse isotropic materials

For the explicit formulation of invariant constitutive equations the representation theorems of tensor functions are used. As discussed in the previous section the governing constitutive equations have to represent the material symmetries of the body of interest a priori. Furthermore, the minimal number of independent scalar variables (the set of independent anisotropic mechanical variables) which have to enter the constitutive expression is required. For a detailed discussion of this topic we refer to Boehler (1987).

### 3.1. Polynomial basis

For the construction of specific constitutive equations we need the invariants of the deformation tensor and the additional structural tensor. An irreducible polynomial basis consists of a collection of members, where none of them can be expressed as a polynomial function of the others. Based on the Hilbert-theorem there exists for a finite basis of tensors a finite integrity basis (see Weyl, 1946). Transverse isotropy is characterized by one preferred unit direction $\boldsymbol{a}$ and the material symmetry group is defined by

$$\mathscr{G}_{\mathrm{ti}} := \{\boldsymbol{I}; \boldsymbol{Q}(\alpha, \boldsymbol{a}) | 0 < \alpha < 2\pi\}, \tag{3.13}$$

where $\boldsymbol{Q}(\alpha, \boldsymbol{a})$ are all rotations about the $\boldsymbol{a}$-axis. The structural tensor $\boldsymbol{M}$ whose invariance group preserves the material symmetry group $\mathscr{G}_{\mathrm{ti}}$ is given by

$$\boldsymbol{M} := \boldsymbol{a} \otimes \boldsymbol{a}. \tag{3.14}$$

The mathematical properties of the structural tensor $\boldsymbol{M}$ are given in Appendix A, Lemma A.12. The integrity bases consist of the traces of products of powers of the argument tensors, the so-called principal invariants and the mixed invariants. The principal invariants $I_k = \hat{I}_k(\boldsymbol{C})$, $k = 1, 2, 3$ of a second order tensor $\boldsymbol{C}$ are defined as the coefficients of the characteristic polynomial

$$f(\lambda) = \det[\lambda \mathbf{1} - \boldsymbol{C}] = \sum_{k=0}^{3} (-1)^k I_k \lambda^{n-k}, \tag{3.15}$$

with $I_0 = 1$ (see also Appendix A, Theorem A.8 and Lemmas A.9 and A.10). The principal invariants of the considered second order tensor have the explicit expressions

$$I_1 := \mathrm{tr}\boldsymbol{C}, \quad I_2 := \mathrm{tr}[\mathrm{Cof}\,\boldsymbol{C}], \quad I_3 := \det \boldsymbol{C}. \tag{3.16}$$

These invariants can also be expressed in terms of the so-called basic invariants $J_i$, $i = 1, 2, 3$. They are defined by the traces of powers of $\boldsymbol{C}$, i.e.

$$J_1 := \mathrm{tr}\boldsymbol{C}, \quad J_2 := \mathrm{tr}[\boldsymbol{C}^2], \quad J_3 := \mathrm{tr}[\boldsymbol{C}^3]. \tag{3.17}$$

These quantities are related to the principal invariants by the simple algebraic expressions

$$J_1 = I_1, \quad J_2 = I_1^2 - 2I_2, \quad J_3 = I_1^3 - 3I_1I_2 + 3I_3. \tag{3.18}$$

The additional invariants, the so-called mixed invariants, to the invariants of a single tensor for two symmetric second order tensors $\boldsymbol{C}$ and $\boldsymbol{M}$ are

$$J_4 := \mathrm{tr}[\boldsymbol{C}\boldsymbol{M}], \quad J_5 := \mathrm{tr}[\boldsymbol{C}^2\boldsymbol{M}], \quad J_6 := \mathrm{tr}[\boldsymbol{C}\boldsymbol{M}^2], \quad J_7 := \mathrm{tr}[\boldsymbol{C}^2\boldsymbol{M}^2], \tag{3.19}$$

(see e.g. Spencer, 1971, 1987). Let $\boldsymbol{M}$ be of rank one and let us assume the normalization condition $\|\boldsymbol{M}\| = 1$, then we obtain the identities $J_6 \equiv J_4$ and $J_7 \equiv J_5$ and we can rule out the terms $J_6$ and $J_7$ from our considerations. The only remaining basic invariant of the single tensor $\boldsymbol{M}$ under the latter condition is

$$\bar{I}_M := \mathrm{tr}\boldsymbol{M}, \tag{3.20}$$

which is a constant. Note that the higher principal invariants of $\boldsymbol{M}$, i.e. $\mathrm{tr}[\mathrm{Cof}\boldsymbol{M}]$ and $\det \boldsymbol{M}$, are equal to zero. Basic properties of the scalar product and tensor product are given in Appendix A, Corollary A.2 and Lemma A.4, respectively. For the construction of constitutive equations it is necessary to determine the minimal set of invariants from which all other invariants can be generated. Here we focus on polynomial invariants. The integrity basis is defined by the set of polynomial invariants which allows the construction of any polynomial invariant as a polynomial in members of the given set (see e.g. Spencer, 1971). The polynomial basis for the construction of a specific free energy function $\psi$ is given by

$$\mathscr{P}_1 := \{I_1, I_2, I_3, J_4, J_5; \bar{I}_M\} \quad \text{or} \quad \mathscr{P}_2 := \{J_1, \ldots, J_5; \bar{I}_M\}. \tag{3.21}$$

The bases (3.21) are invariant under all transformations with elements of $\mathscr{G}_{\mathrm{ti}}$. As a result the polynomial functions in elements of the polynomial basis are also invariant under these transformations. For the free energy function we assume the general form

$$\psi = \hat{\psi}(L_i | L_i \in \mathscr{P}_j) + c \quad \text{for } j = 1 \text{ or } j = 2. \tag{3.22}$$

In order to fulfill the non-essential normalization condition $\psi(\mathbf{1}) = 0$ we introduce the constant $c \in \mathbb{R}$.

### 3.2. Representation of polyconvex free energy functions

In this section we discuss specific forms of the free energy function $\psi$ for transverse isotropy in order to guarantee the existence of minimizers of some variational principles for finite strains. The existence of minimizers of some variational principles in finite elasticity is based on the concept of quasiconvexity, introduced by Morrey (1952), which ensures that the functional to be minimized is weakly lower semi-continuous. This inequality condition is rather complicated to handle since it is an integral inequality. Thus a more important concept for practical use is the notion of polyconvexity in the sense of Ball (1977a,b) in this context see also Marsden and Hughes (1983) and Ciarlet (1988). For isotropic material response functions there exist some models, e.g. the Ogden-, Mooney-Rivlin- and Neo-Hooke-type models, which satisfy this concept. Furthermore, it can be shown that polyconvexity of the stored energy implies that the corresponding acoustic tensor is elliptic for all deformations. For finite-valued, continuous functions we can recapitulate the important implications:

convexity $\Rightarrow$ polyconvexity $\Rightarrow$ quasiconvexity $\Rightarrow$ rank one convexity.

The converse implications are not true. Furthermore, the quasiconvexity of a function ensures that the associated functional to be minimized is weakly lower semi-continuous and the rank one convexity of a function ensures that the Euler equations of the associated functional are elliptic (in this context see e.g. Dacorogna, 1989 and Silhavý, 1977).

Now we introduce $W \in C^2(\mathbb{M}^{3\times3}, \mathbb{R})$, a given scalar valued energy density. We say that

**Definition 3.1** (*Polyconvexity*). $\boldsymbol{F} \mapsto W(\boldsymbol{F})$ is polyconvex if and only if there exists a function $P : \mathbb{M}^{3\times3} \times \mathbb{M}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ (in general non-unique) such that

$$W(\boldsymbol{F}) = P(\boldsymbol{F}, \mathrm{Adj}\,\boldsymbol{F}, \det \boldsymbol{F})$$

and the function $\mathbb{R}^{19} \mapsto \mathbb{R}, (\widetilde{X}, \widetilde{Y}, \widetilde{Z}) \mapsto P(\widetilde{X}, \widetilde{Y}, \widetilde{Z})$ is convex for all points $\boldsymbol{X} \in \mathbb{R}^3$.

In the above definition and in the following we drop the $\boldsymbol{X}$-dependence of the individual functions if there is no danger of confusion, i.e. we write $W \in C^2(\mathbb{M}^{3\times3}, \mathbb{R})$ instead of $W \in C^2(\mathbb{R}^3 \times \mathbb{M}^{3\times3}, \mathbb{R})$ and $P : \mathbb{M}^{3\times3} \times \mathbb{M}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ instead of $P : \mathbb{R}^3 \times \mathbb{M}^{3\times3} \times \mathbb{M}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ in order to arrive at a more compact notation. The definition of the adjugate of $\boldsymbol{F} \in \mathbb{M}^{3\times3}$ is given in Appendix A, A5–A7 and the properties of the adjugate are listed in Appendix A, Lemma A.6.

A consequence of the Definition 3.1 for a more restrictive class of energy densities is

**Corollary 3.2** (Additive polyconvex functions). *Let* $W(\boldsymbol{F}) = W_1(\boldsymbol{F}) + W_2(\mathrm{Adj}\,\boldsymbol{F}) + W_3(\det \boldsymbol{F})$. *If* $W_i$, $i = 1, 2$ *are convex in the associated variable respectively and* $W_3 : \mathbb{R}^+ \mapsto \mathbb{R}$ *is convex in the associated variable as well, then* $W$ *is altogether polyconvex.*

The last corollary will be one of our primary tools in constructing polyconvex strain energy functions: we identify convex functions on $\mathbb{M}^{3\times3}$ and $\mathbb{R}$ and then take positive combinations of them.

Let $\boldsymbol{w} \in C_0^\infty(\mathscr{B})$ denote the set of infinitely differential functions $\boldsymbol{w}$ that vanish on $\partial\mathscr{B}$.

**Definition 3.3** (*Quasiconvexity*). The elastic free energy is quasiconvex whenever for all $\mathscr{B} \subset \mathbb{R}^3$ and all $\boldsymbol{F} \in \mathbb{M}^{3\times3}$ and all $\boldsymbol{w} \in C_0^\infty(\mathscr{B})$ we have

$$W(\boldsymbol{F})|\mathscr{B}| = \int_{\mathscr{B}} W(\boldsymbol{F})\,\mathrm{d}V \leqslant \int_{\mathscr{B}} W(\boldsymbol{F} + \nabla \boldsymbol{w})\,\mathrm{d}V.$$

**Definition 3.4** (*Ellipticity*). We say that the elastic free energy $W(\boldsymbol{F}) = \psi(\boldsymbol{C}) \in C^2(\mathbb{M}^{3\times3}, \mathbb{R})$ leads to a uniformly elliptic equilibrium system whenever the so-called uniform Legendre-Hadamard condition

$$\exists c^+ > 0\ \forall \boldsymbol{F} \in \mathbb{M}^{3\times3} : \forall \xi, \eta \in \mathbb{R}^3 : \quad D_F^2 W(\boldsymbol{F}).(\xi \otimes \eta, \xi \otimes \eta) \geqslant c^+ \|\xi\|^2 \|\eta\|^2$$

holds. We say that $W$ leads to an elliptic system if and only if the Legendre-Hadamard condition

$$\forall \boldsymbol{F} \in \mathbb{M}^{3\times3} : \forall \xi, \eta \in \mathbb{R}^3 : \quad D_F^2 W(\boldsymbol{F}).(\xi \otimes \eta, \xi \otimes \eta) \geqslant 0$$

holds. We say that the elastic free energy $W$ is rank-one convex if the function $f : \mathbb{R} \mapsto \mathbb{R}$, $f(t) = W(\boldsymbol{F} + t(\xi \otimes \eta))$ is convex for all $\boldsymbol{F} \in \mathbb{M}^{3\times3}$ and all $\xi, \eta \in \mathbb{R}^3$.

The decisive property in the context to be treated here is the following well-known property:

**Theorem 3.5** (Polyconvexity implies ellipticity). *Let* (*i*) *W be polyconvex. Then W is elliptic. Let* (*ii*) *W be sufficiently smooth. Then rank-one convexity and ellipticity are equivalent.*

The proof of the last theorem is based on standard results in the calculus of variations (see e.g. Dacorogna, 1989). We remark that the converse is not true.

To obtain various strain energy terms in order to model specific problems, which permit the matching of data stemming from experiments we assume an additively decoupled structure of $\psi$, i.e.

$$\psi = \sum_{j=1}^{n} \hat{\psi}_j(\boldsymbol{C}, \boldsymbol{M}) = \sum_{j=1}^{n} \hat{\psi}_j(\boldsymbol{C}, \mathrm{Cof}\,\boldsymbol{C}, \det\,\boldsymbol{C}, \boldsymbol{M}). \tag{3.23}$$

The formal representation (3.23) second part is of interest with respect to the construction of alternative polynomial bases; this will be discussed in the following sections. We demand that each term $\psi_j | j = 1, ..n$ has to satisfy a priori the invariance conditions and the polyconvexity condition. It should be noted that the formal similarity in the list of arguments (3.23 second part), i.e. $(\boldsymbol{C}, \mathrm{Cof}\,\boldsymbol{C}, \bullet)$, with the argument of the convex function $P : \mathbb{M}^{3\times3} \times \mathbb{M}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ of definition 3.1, i.e. $(\boldsymbol{F}, \mathrm{Adj}\,\boldsymbol{F}, \bullet)$, is a consequence of the material objectivity condition. However, it does not suppose any convexity requirements with respect to $(\boldsymbol{C}, \operatorname{Cof}\boldsymbol{C}, \bullet)$ of course. In the following, we first concentrate on isotropic functions, point out some relations to well-known formulations and then focus on anisotropic terms. The additively decoupled formulation (3.23) in the individual invariants leads with (2.6) to the stress response function

$$\boldsymbol{S} = 2\frac{\partial\psi}{\partial\boldsymbol{C}} = 2\sum_{j=1}^{n}\sum_{L_i\in\mathscr{P}_1\backslash\bar{I}_M}\frac{\partial\psi_j}{\partial L_i}\frac{\partial L_i}{\partial\boldsymbol{C}}. \tag{3.24}$$

The tensor generators $\partial_C L_i$ are independent of the specific form of the free energy function. They only depend on the symmetry of the material characterized by the introduced structural tensors. Although the symmetry group for transverse isotropy is completely characterized by the invariance group of $\boldsymbol{M}$, defined in (3.14), we introduce an additional dependent structural tensor,

$$\boldsymbol{D} := \boldsymbol{1} - \boldsymbol{M}. \tag{3.25}$$

By a simple calculation we see directly that the invariance group of $\boldsymbol{D}$ is the material symmetry group $\mathscr{G}_{\text{ti}}$. Thus $\boldsymbol{D}$ is a possible structural tensorial quantity instead of $\boldsymbol{M}$. The introduction of this additional quantity is useful for a comprehensive representation and physical interpretation of several terms of the free energy function.

#### 3.2.1. Isotropic free energy terms

In this section we analyse some isotropic free energy functions which fulfill the polyconvexity condition. Furthermore, we point out some results for well-known functions. It is sometimes preferable to express strain energies as a sum of isochoric and volumetric terms. Let $\boldsymbol{F} \in GL(3,\mathbb{R})$, then we obtain with (2.2)

$$\widetilde{\boldsymbol{C}} := \boldsymbol{C}/I_3^{\frac{1}{3}} \quad \text{with } \det[\widetilde{\boldsymbol{C}}] = 1. \tag{3.26}$$

The ansatz for a free energy function is assumed to be of the form

$$W(\boldsymbol{F}) = W_{\text{iso}}(\widetilde{\boldsymbol{C}}) + W_{\text{vol}}(\det\boldsymbol{F}). \tag{3.27}$$

We will show that this ansatz is compatible with the requirement of polyconvexity. Let for example $W_1(A) = \langle\boldsymbol{H}, \boldsymbol{1}\rangle$ and define $\text{iso}(\boldsymbol{F}) = \widetilde{\boldsymbol{C}}$. Then

$$W_{\text{iso}}(\widetilde{\boldsymbol{C}}) = W_1(\text{iso}(\boldsymbol{F})) = \begin{cases} \frac{\|\boldsymbol{F}\|^2}{(\det\boldsymbol{F})^{\frac{2}{3}}} & \text{for } \det\boldsymbol{F} > 0 \\ \infty & \text{for } \det\boldsymbol{F} \leqslant 0 \end{cases} \tag{3.28}$$

and $W(\boldsymbol{F}) = W_1(\text{iso}(\boldsymbol{F}))$ is a polyconvex function (however not of the additive type, Corollary 3.2) which we proceed to show in Appendix C, Lemma C.1. For the remainder let us agree to extend functions $W$, which are naturally only defined on the set $\det\boldsymbol{F} > 0$ to $\mathbb{M}^{3\times3}$ by setting $W = \infty$ for arguments with $\det\boldsymbol{F} \leqslant 0$ as we did in the last example. It is clear by such an extension that $W$ can never be convex, for it is supported on a non-convex set only. However, this extension is compatible with the requirement of polyconvexity since

$$P(x) = \begin{cases} f(x) & x > 0 \\ \infty & x \leqslant 0 \end{cases} \tag{3.29}$$

is a convex function whenever $f$ is convex on $\mathbb{R}^+$. Some polyconvex, isotropic free energy terms which we will use for the identification with the linearized standard moduli at the reference configuration and for the simulations are

$$\psi_1 := \alpha_1 I_1, \quad \psi_2 := \alpha_2 I_1^2, \quad \psi_3 := \alpha_3\frac{I_1}{I_3^{1/3}}, \quad \psi_4 := \alpha_4\frac{I_1^2}{I_3^{1/3}} \tag{3.30}$$

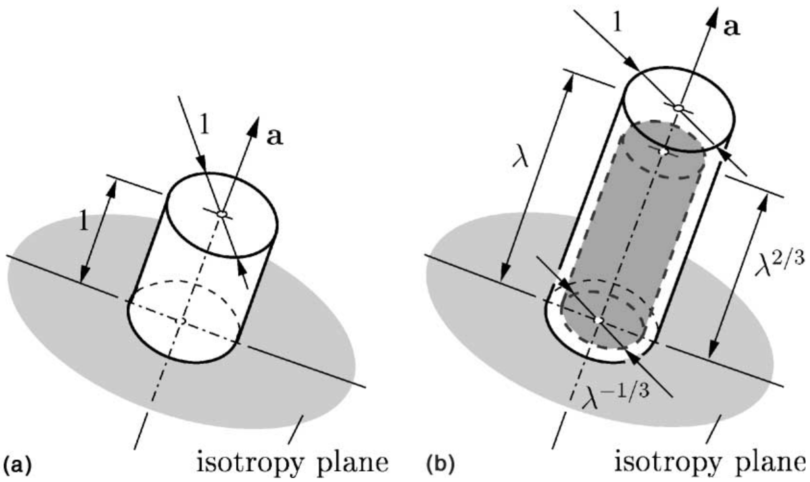


Fig. 2. Physical interpretation of the polyconvex invariant function $I_1/I_3^{1/3}$.

with all $\alpha_i > 0$. The first and second terms are powers of traces of the right Cauchy–Green tensor, while the third one is an isochoric term and the last one is the product of the functions of the invariant expressions appearing in $\psi_1$ and $\psi_3$.

For the physical interpretation of the isotropic invariant function $I_1/I_3^{1/3}$ we consider a cylinder of unit length and unit diameter (see Fig. 2a). A deformation described by the deformation gradient $\boldsymbol{F} = \mathbf{1} + (\lambda - 1)\boldsymbol{a} \otimes \boldsymbol{a}$, with $\|\boldsymbol{a}\| = 1$, leads to a final configuration as outlined by the outer cylinder in Fig. 2b. The isochoric part of $\boldsymbol{F}$, i.e. the term $\widetilde{\boldsymbol{F}} := (\det \boldsymbol{F})^{-1/3}\boldsymbol{F}$, and thus the quadratic function in the remainder $I_1/I_3^{1/3} = \operatorname{tr}\widetilde{\boldsymbol{C}} = \|\widetilde{\boldsymbol{F}}\|^2$, controls only the isochoric part of the deformation. In the considered example only the shaded volume in Fig. 2b is affected by this invariant. For the anisotropic case we will discuss this from a different point of view.

The convexity of $I_1^k$, i.e. $\boldsymbol{F} \mapsto [\operatorname{tr}(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F})]^k$, $k \geqslant 1$ can be proved by the positivity of the second derivative.

**Proof.** (1) With the identity $[\operatorname{tr}(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F})]^k = \|\boldsymbol{F}\|^{2k}$ we obtain

$$D_F\left(\|\boldsymbol{F}\|^{2k}\right).\boldsymbol{H} = 2k\|\boldsymbol{F}\|^{2k-2}\langle \boldsymbol{F}, \boldsymbol{H}\rangle$$

$$D_F^2\left(\|\boldsymbol{F}\|^{2k}\right).(\boldsymbol{H}, \boldsymbol{H}) = 2k\left(\|\boldsymbol{F}\|^{2k-2}\langle \boldsymbol{H}, \boldsymbol{H}\rangle + (2k-2)\|\boldsymbol{F}\|^{2k-4}\langle \boldsymbol{F}, \boldsymbol{H}\rangle^2\right) > 0.$$

The proof of the polyconvexity of the terms $I_1^k/I_3^{1/3}$ for $k \geqslant 1$ is given in Lemma C.3, Eq. (1) (see the Appendix). In an analogous manner we construct free energy terms in the second principal invariant $I_2$. For the following analysis we choose the four terms

$$\psi_5 := \eta_1 I_2, \quad \psi_6 := \eta_2 I_2^2, \quad \psi_7 := \eta_3 \frac{I_2}{I_3^{1/3}}, \quad \psi_8 := \eta_4 \frac{I_2^2}{I_3^{1/3}} \tag{3.31}$$

with $\eta_i \geqslant 0$. The interpretation of these terms is similar to the functions presented in (3.30) with the modification that the surface deformation of the considered infinitesimal volume element is controlled; this can be seen directly by $I_2 = \operatorname{tr}\operatorname{Cof}\boldsymbol{C} = \|\operatorname{Cof}\boldsymbol{F}\|^2$ and taking (2.3 first part) into account. The proof of polyconvexity of (3.31) is straightforward by replacing $\boldsymbol{F}$ with $\operatorname{Cof}\boldsymbol{F}$ in Proof (1). Furthermore, terms in traces of powers of $\boldsymbol{C}$ are also convex, i.e.

$$\boldsymbol{F} \mapsto \mathrm{tr}[(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F})^k] \quad \text{with } k \geqslant 1$$

is a convex mapping. This function allows the direct usage of the basic invariants (3.17) for the construction of polyconvex free energy functions.

**Proof.** (2) Set $\boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}$, then the first and second derivatives with respect to $\boldsymbol{C}$ are

$$D_C\big(\mathrm{tr}[\boldsymbol{C}^k]\big).\boldsymbol{H} = D_C\big(\langle \boldsymbol{C}^k, \mathbb{1}\rangle\big).\boldsymbol{H} = k\langle \boldsymbol{C}^{k-1}, \boldsymbol{H}\rangle,$$

$$D_C^2\big(\mathrm{tr}[\boldsymbol{C}^k]\big).(\boldsymbol{H},\boldsymbol{H}) = k(k-1)\langle \boldsymbol{C}^{k-2}\boldsymbol{H}, \boldsymbol{H}\rangle \geqslant 0.$$

Thus $D_C(\mathrm{tr}[\boldsymbol{C}^k]) = k\boldsymbol{C}^{k-1} \in P\mathbb{S}\mathrm{ym}$ and $D_C^2(\mathrm{tr}[\boldsymbol{C}^k]).(\boldsymbol{H},\boldsymbol{H}) \geqslant 0$ which allows us to apply Lemma B.5; in this regard see the Appendix. □

As examples for some volumetric terms in $\det \boldsymbol{F}$ or $\det \boldsymbol{C}$ we consider the expressions

$$\begin{aligned} &\psi_9 := \delta_1 I_3, \quad \psi_{10} := -\delta_2 \ln \sqrt{I_3}, \quad \psi_{11} := \delta_3\left(I_3 + \frac{1}{I_3}\right), \\ &\psi_{12} := \delta_4 (I_3 - 1)^2, \quad \psi_{13} := \delta_5 \frac{1}{I_3} \end{aligned} \tag{3.32}$$

with $\delta_i \geqslant 0$. Further examples for polyconvex volumetric free energy terms are

$$\left.\begin{array}{ll} \boldsymbol{F} \mapsto \left(\det \boldsymbol{C} + \frac{1}{\det \boldsymbol{C}} - 2\right)^k & \text{with } k \geqslant 1 \\ \boldsymbol{F} \mapsto \left((\det \boldsymbol{C})^p + \frac{1}{(\det \boldsymbol{C})^p} - 2\right)^k & \text{with } k \geqslant 1, p \geqslant \frac{1}{2} \\ \boldsymbol{F} \mapsto (\sqrt{\det \boldsymbol{C}} - 1)^k & \text{with } k \geqslant 1 \\ \boldsymbol{F} \mapsto (\det \boldsymbol{C} - \ln[\det \boldsymbol{C}]) & \\ \boldsymbol{F} \mapsto (\det \boldsymbol{C} - \ln[\det \boldsymbol{C}] + (\ln[\det \boldsymbol{C}])^2) & \end{array}\right\}. \tag{3.33}$$

On the natural domain of definition $\det \boldsymbol{F} > 0$ the given functions are convex in the variable $\det \boldsymbol{F}$. The terms in (3.33) are each polyconvex and lead to a stress free reference configuration. Furthermore, the following isochoric terms are polyconvex and stress free in the natural state:

$$\left.\begin{array}{ll} \boldsymbol{F} \mapsto \left(\dfrac{\|\boldsymbol{F}\|^{2k}}{(\det \boldsymbol{F})^{\frac{2k}{3}}} - 3^k\right)^i & \text{with } i \geqslant 1, k \geqslant 1 \\ \boldsymbol{F} \mapsto \left(\dfrac{\|\mathrm{Adj}\,\boldsymbol{F}\|^{3k}}{(\det \boldsymbol{F})^{2k}} - (3\sqrt{3})^k\right)^j & \text{with } j \geqslant 1, k \geqslant 1 \\ \boldsymbol{F} \mapsto \exp\left[\left(\dfrac{\|\boldsymbol{F}\|^{2k}}{(\det \boldsymbol{F})^{\frac{2k}{3}}} - 3^k\right)^i\right] - 1 & \text{with } i \geqslant 1, k \geqslant 1 \\ \boldsymbol{F} \mapsto \exp\left[\left(\dfrac{\|\mathrm{Adj}\,\boldsymbol{F}\|^{3k}}{(\det \boldsymbol{F})^{2k}} - (3\sqrt{3})^k\right)^j\right] - 1 & \text{with } j \geqslant 1, k \geqslant 1 \end{array}\right\}. \tag{3.34}$$

For the proof of this statement see the Appendix, Lemma C.5 and Corollary C.6. The treatment of the isotropic case has been taken from Hartmann and Neff (2002). For the explicit derivations of the stress functions and the moduli we choose from (3.34) the terms

$$\psi_{14} := \omega_1 \left( \frac{I_1}{I_3^{1/3}} - 3 \right)^2, \quad \psi_{15} := \omega_2 \left( \frac{I_2^3}{I_3^2} - (3\sqrt{3})^2 \right)$$
$$\psi_{16} := \omega_3 \left( \exp\left[ \frac{I_1}{I_3^{1/3}} - 3 \right] - 1 \right), \quad \psi_{17} := \omega_4 \left( \exp\left[ \frac{I_2^3}{I_3^2} - (3\sqrt{3})^2 \right] - 1 \right) \tag{3.35}$$

with $\omega_i \geqslant 0$. The above isotropic terms of the type

$$W(\boldsymbol{F}) = \left( \frac{\|\boldsymbol{F}\|^2}{(\det \boldsymbol{F})^{\frac{2}{3}}} - 3 \right)^i \quad \text{with } i \geqslant 1$$

have the convenient property that $W(\mathbf{1}) = 0$ in the unstressed configuration and $W(\boldsymbol{F}) \geqslant 0$. Hence the reference configuration is automatically stress-free. This contrasts with known polyconvex functions such as compressible Mooney-Rivlin materials, where only by a judicious choice of parameters can the reference configuration be made stress-free. The polyconvexity of these terms is shown in Hartmann and Neff (2002). Of course, the terms are objective and meet various growth conditions necessary for the successful application of the direct methods of variations to prove the existence of solutions for a corresponding finite elasticity boundary value problem.

The stresses related to the above free energy terms can be obtained by exploiting (3.24). All terms are formulated in the principal invariants $I_1$, $I_2$, $I_3$, so we arrive at

$$\boldsymbol{S}_1 := 2 \sum_{j=1}^{n} \left\{ \frac{\partial \psi_j}{\partial I_1} \frac{\partial I_1}{\partial \boldsymbol{C}} + \frac{\partial \psi_j}{\partial I_2} \frac{\partial I_2}{\partial \boldsymbol{C}} + \frac{\partial \psi_j}{\partial I_3} \frac{\partial I_3}{\partial \boldsymbol{C}} \right\}. \tag{3.36}$$

With the derivatives of the principal invariants with respect to $\boldsymbol{C}$, which are given by

$$\left.\begin{aligned} \frac{\partial I_1}{\partial \boldsymbol{C}} &= \boldsymbol{G}^{-1} \\ \frac{\partial I_3}{\partial \boldsymbol{C}} &= \det[\boldsymbol{C}]\boldsymbol{C}^{-1} \\ \frac{\partial I_2}{\partial \boldsymbol{C}} &= \frac{\partial(\det[\boldsymbol{C}]\mathrm{tr}[\boldsymbol{C}^{-1}])}{\partial \boldsymbol{C}} = \mathrm{tr}[\boldsymbol{C}^{-1}] \det[\boldsymbol{C}]\boldsymbol{C}^{-1} - \det[\boldsymbol{C}]\boldsymbol{C}^{-2} \end{aligned}\right\}, \tag{3.37}$$

we obtain with $\mathrm{Cof}\,\boldsymbol{C} = \det[\boldsymbol{C}]\boldsymbol{C}^{-1}$ the stresses in the form

$$\boldsymbol{S}_1 = 2 \sum_{j=1}^{n} \left\{ \frac{\partial \psi_j}{\partial I_1} \boldsymbol{G}^{-1} + \frac{\partial \psi_j}{\partial I_2} (\mathrm{tr}[\boldsymbol{C}^{-1}]\mathrm{Cof}[\boldsymbol{C}] - \boldsymbol{C}^{-1}\mathrm{Cof}[\boldsymbol{C}]) + \frac{\partial \psi_j}{\partial I_3} \mathrm{Cof}\,\boldsymbol{C} \right\}. \tag{3.38}$$

Multiplying the Cayley-Hamilton theorem for the characteristic polynomial of the argument tensor with $\boldsymbol{C}^{-1}$ leads with $\mathrm{tr}[\mathrm{Cof}\,\boldsymbol{C}] = \mathrm{tr}\boldsymbol{C}^{-1} \det \boldsymbol{C}$ to the expression

$$\mathrm{tr}[\boldsymbol{C}^{-1}]\mathrm{Cof}[\boldsymbol{C}] - \boldsymbol{C}^{-1}\mathrm{Cof}[\boldsymbol{C}] = \mathrm{tr}[\boldsymbol{C}]\boldsymbol{G}^{-1} - \boldsymbol{G}^{-1}\boldsymbol{C}\boldsymbol{G}^{-1}, \tag{3.39}$$

which simplifies (3.38). In this manner we arrive at the representation

$$\boldsymbol{S}_1 = 2 \sum_{j=1}^{n} \left\{ \left( \frac{\partial \psi_j}{\partial I_1} + \frac{\partial \psi_j}{\partial I_2} I_1 \right) \boldsymbol{G}^{-1} - \frac{\partial \psi_j}{\partial I_2} \boldsymbol{G}^{-1}\boldsymbol{C}\boldsymbol{G}^{-1} + \frac{\partial \psi_j}{\partial I_3} \mathrm{Cof}\,\boldsymbol{C} \right\}. \tag{3.40}$$

The material tangent moduli are denoted in index-representation by $\mathbb{C}_1^{ABCD} := 2\partial_{C_{CD}} S_1^{AB}$. Based on the formula (3.40) we arrive with $\partial^2\psi/(\partial I_i \partial I_j) = \partial^2\psi/(\partial I_j \partial I_i)$ at

$$\mathbb{C}_1^{ABCD} = 4\sum_{j=1}^{n}\left[\frac{\partial^2\psi_j}{\partial I_1\,\partial I_1}\boldsymbol{G}^{AB}\boldsymbol{G}^{CD} + \frac{\partial^2\psi_j}{\partial I_2\,\partial I_2}\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{AB}\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{CD} + \frac{\partial^2\psi_j}{\partial I_3\,\partial I_3}\{\mathrm{Cof}\,\boldsymbol{C}\}^{AB}\{\mathrm{Cof}\,\boldsymbol{C}\}^{CD}\right.$$
$$+\frac{\partial^2\psi_j}{\partial I_2\,\partial I_1}[\boldsymbol{G}^{AB}\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{CD} + \{I_1\boldsymbol{G}-\boldsymbol{C}\}^{AB}\boldsymbol{G}^{CD}] + \frac{\partial^2\psi_j}{\partial I_3\,\partial I_1}[\boldsymbol{G}^{AB}\{\mathrm{Cof}\,\boldsymbol{C}\}^{CD} + \{\mathrm{Cof}\,\boldsymbol{C}\}^{AB}\boldsymbol{G}^{CD}]$$
$$+\frac{\partial^2\psi_j}{\partial I_3\,\partial I_2}[\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{AB}\{\mathrm{Cof}\,\boldsymbol{C}\}^{CD} + \{\mathrm{Cof}\,\boldsymbol{C}\}^{AB}\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{CD}] + \frac{\partial\psi_j}{\partial I_2}[\boldsymbol{G}^{AB}\boldsymbol{G}^{CD} - \boldsymbol{G}^{AC}\boldsymbol{G}^{BD}]$$
$$\left.+\frac{\partial\psi_j}{\partial I_3}I_3[\{\boldsymbol{C}^{-1}\}^{AB}\{\boldsymbol{C}^{-1}\}^{CD} - \{\boldsymbol{C}^{-1}\}^{AC}\{\boldsymbol{C}^{-1}\}^{BD}]\right]. \tag{3.41}$$

In (3.41) $\{\boldsymbol{C}\}^{CD}$ is an abbreviation for the index representation of $\boldsymbol{G}^{-1}\boldsymbol{C}\boldsymbol{G}^{-1}$ in order to arrive at a compact formulation.

### 3.2.2. Anisotropic free energy terms

For the anisotropic part we construct several terms in an analogous way to that pointed out above, see also Schröder and Neff (2001). Before starting the construction and discussion of several polyconvex, transversely isotropic functions we have a look at often-used direct extensions of the small strain theory to the case of finite deformations by substituting the linear strain tensor with the Green–Lagrange strain tensor $\boldsymbol{E} := \frac{1}{2}(\boldsymbol{C}-\boldsymbol{G})$. A typical form of such an extension is the quadratic function in $\boldsymbol{E}$ e.g.

$$\psi_E := \tilde{c}_1(\mathrm{tr}\boldsymbol{E})^2 + \tilde{c}_2\mathrm{tr}[\boldsymbol{E}^2] + \tilde{c}_3\mathrm{tr}\boldsymbol{E}\,\mathrm{tr}[\boldsymbol{M}\boldsymbol{E}] + \tilde{c}_4(\mathrm{tr}[\boldsymbol{M}\boldsymbol{E}])^2 + \tilde{c}_5\mathrm{tr}[\boldsymbol{M}\boldsymbol{E}^2]. \tag{3.42}$$

Since formulations like (3.42) in $\boldsymbol{E}$ are a priori not polyconvex and not elliptic, we consider a different formulation in the right Cauchy–Green tensor which has some superficially similar characteristics to $\psi_E$. So let us consider the quadratic free energy function in terms of the elements of a polynomial basis in $\boldsymbol{C}$ and $\boldsymbol{M}$, i.e.

$$\psi_C := \bar{c}_1 I_1^2 + \bar{c}_2 J_2 + \bar{c}_3 I_1 J_4 + \bar{c}_4 J_4^2 + \bar{c}_5 J_5 + \bar{c}_6 f_G + \bar{c}_7 f_M, \tag{3.43}$$

where $f_G$ and $f_M$ are functions which we introduce in order to fulfill the condition of a stress-free reference configuration with respect to the tensor generators $\boldsymbol{G}^{-1}$ and $\boldsymbol{M}$, respectively. The first and second terms are polyconvex, see the proofs in the last section. The term $I_1J_4$ does not fulfill the polyconvexity condition, i.e. the expression

$$\boldsymbol{F} \mapsto \mathrm{tr}(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}\boldsymbol{M})\mathrm{tr}(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}) = \mathrm{tr}[\boldsymbol{C}\boldsymbol{M}]\mathrm{tr}\boldsymbol{C} = I_1J_4$$

is not polyconvex, because it is not even elliptic and hence not quasiconvex.

**Proof.** (3) The last equation can be expressed in the form

$$\mathrm{tr}[\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}\boldsymbol{M}]\mathrm{tr}[\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}] = \|\boldsymbol{F}\|^2\|\boldsymbol{F}\boldsymbol{a}\|^2_{\mathbb{R}^3}.$$

Calculating the second differential with respect to the deformation gradient yields

$$D_F^2(\|\boldsymbol{F}\|^2\|\boldsymbol{F}\boldsymbol{a}\|^2_{\mathbb{R}^3}).(\boldsymbol{H},\boldsymbol{H}) = 8\langle\boldsymbol{F},\boldsymbol{H}\rangle\langle\boldsymbol{F}\boldsymbol{a},\boldsymbol{H}\boldsymbol{a}\rangle_{\mathbb{R}^3} + 2\|\boldsymbol{F}\boldsymbol{a}\|^2_{\mathbb{R}^3}\|\boldsymbol{H}\|^2 + 2\|\boldsymbol{F}\|^2\|\boldsymbol{H}\boldsymbol{a}\|^2_{\mathbb{R}^3}.$$

We see that this expression is in general non-positive (take $\boldsymbol{F}$, $\boldsymbol{H}$ in diagonal form), which excludes convexity. However, it is possible to show the non-ellipticity as well. Take

$$\boldsymbol{F}_n := \begin{pmatrix} \frac{1}{n} & -1 & 0 \\ 0 & \frac{1}{n} & 0 \\ 0 & 0 & \frac{1}{n} \end{pmatrix}, \quad \xi = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \eta = \begin{pmatrix} 1 \\ n \\ 0 \end{pmatrix}, \quad \boldsymbol{a} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

and $\boldsymbol{H} = \xi \otimes \eta$. This yields

$$D^2_F(\|\boldsymbol{F}\|^2\|\boldsymbol{F}\boldsymbol{a}\|^2_{\mathbb{R}^3}).(\xi \otimes \eta, \xi \otimes \eta) = 8\langle \boldsymbol{F}, \xi \otimes \eta\rangle\langle \boldsymbol{F}\boldsymbol{a}, \xi \otimes \eta \boldsymbol{a}\rangle_{\mathbb{R}^3} + 2\|\boldsymbol{F}\boldsymbol{a}\|^2_{\mathbb{R}^3}\|\xi \otimes \eta\|^2 + 2\|\boldsymbol{F}\|^2\|\xi \otimes \eta \boldsymbol{a}\|^2_{\mathbb{R}^3}$$
$$= 8\left(\frac{1}{n} - n\right)\frac{1}{n} + 2\frac{1}{n^2}\,(1+n^2) + 2\left(3\frac{1}{n^2} + 1\right) = \frac{16}{n^2} - 4.$$

If we choose $n > 2$, then we get

$$D^2_F(\|\boldsymbol{F}\|^2\|\boldsymbol{F}\boldsymbol{a}\|^2_{\mathbb{R}^3}).(\xi \otimes \eta, \xi \otimes \eta) < 0.$$

Thus, the non-ellipticity of the function $I_1 J_4$ is shown. □

Now we analyse expressions in powers of the basic invariant $J_4$. The polynomial functions

$$\boldsymbol{F} \mapsto (\text{tr}[\boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{M}])^k = (\text{tr}[\boldsymbol{C}\boldsymbol{M}])^k = J_4^k \quad \text{with } k \geqslant 1$$

are polyconvex. For the proof of this we check the convexity of $J_4^k$ with respect to $\boldsymbol{F}$.

**Proof.** (4) The first and second differential of the expression $(\text{tr}[\boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{M}])^k = \langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^k$ with respect to $\boldsymbol{F}$ are given by

$$D_F\left(\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^k\right).\boldsymbol{H} = k\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^{k-1}(\langle \boldsymbol{F}, \boldsymbol{H}\boldsymbol{M}\rangle + \langle \boldsymbol{H}, \boldsymbol{F}\boldsymbol{M}\rangle) = 2k\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^{k-1}\langle \boldsymbol{F}, \boldsymbol{H}\boldsymbol{M}\rangle$$

$$D^2_F\left(\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^k\right).(\boldsymbol{H}, \boldsymbol{H}) = 4k(k-1)\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^{k-2}\langle \boldsymbol{F}\boldsymbol{M}, \boldsymbol{H}\rangle^2 + 2k\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^{k-1}\langle \boldsymbol{H}, \boldsymbol{H}\boldsymbol{M}\rangle \geqslant 0,$$

respectively. For the evaluation of the single terms see Lemma A.12, Eq. (15). □

In (3.44) we summarized some functions in the invariants $J_4$ and $I_3$ which are polyconvex,

$$\psi_{18} := \beta_1 J_4, \quad \psi_{19} := \beta_2 J_4^2, \quad \psi_{20} := \beta_3 \frac{J_4}{I_3^{1/3}}, \quad \psi_{21} := \beta_4 \frac{J_4^2}{I_3^{1/3}} \tag{3.44}$$

with $\beta_i \geqslant 0$. The term $\psi_{18}$ characterizes the square of the stretch and $\psi_{19}$ the quartic stretch in the preferred direction. With the function $J_4/I_3^{1/3} = \widetilde{\boldsymbol{C}} : \boldsymbol{M}$ we can cover the square of the stretch in direction $\boldsymbol{a}$ due to the isochoric part of the deformation. The last term in (3.44) is not decoupled with respect to the volumetric and isochoric deformations. Other possibilities for higher order terms are given in Lemma C.3, Eq. (2).

Now we analyse terms in the mixed invariant $J_5$. The following term is not elliptic and hence non-quasiconvex:

$$\boldsymbol{F} \mapsto \text{tr}[\boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{M}] = \text{tr}[\boldsymbol{C}^2\boldsymbol{M}] = J_5.$$

**Proof.** (5) The forms of the individual expressions are

$$\text{tr}[\boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{M}] = \|\boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{a}\|^2_{\mathbb{R}^3}.$$

First we compute the second derivative of the function with respect to $\boldsymbol{F}$

$$D^2_F(\|\boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{a}\|^2_{\mathbb{R}^3}).(\boldsymbol{H}, \boldsymbol{H}) = 2\langle \boldsymbol{F}^{\text{T}}\boldsymbol{F}\boldsymbol{a}, \boldsymbol{H}^{\text{T}}\boldsymbol{H}\boldsymbol{a}\rangle_{\mathbb{R}^3} + \|(\boldsymbol{F}^{\text{T}}\boldsymbol{H} + \boldsymbol{H}^{\text{T}}\boldsymbol{F})\boldsymbol{a}\|^2_{\mathbb{R}^3}.$$

Set $\boldsymbol{H} = \xi \otimes \eta$ with $\|\xi\|_{\mathbb{R}^3} = \|\eta\|_{\mathbb{R}^3} = 1$. This yields after some manipulations

$$D_F^2(\|\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}\boldsymbol{a}\|_{\mathbb{R}^3}^2).(\xi \otimes \eta, \xi \otimes \eta) = 2\langle \boldsymbol{F}\boldsymbol{a}, \boldsymbol{F}\eta\rangle_{\mathbb{R}^3}\langle \eta, \boldsymbol{a}\rangle_{\mathbb{R}^3} + \langle \eta, \boldsymbol{a}\rangle_{\mathbb{R}^3}^2\|\boldsymbol{F}^{\mathrm{T}}\xi\|_{\mathbb{R}^3}^2 + \langle \boldsymbol{F}^{\mathrm{T}}\xi, \boldsymbol{a}\rangle_{\mathbb{R}^3}^2 + 2\langle \boldsymbol{F}^{\mathrm{T}}\xi, \eta\rangle_{\mathbb{R}^3}\langle \eta, \boldsymbol{a}\rangle_{\mathbb{R}^3}\langle \boldsymbol{F}^{\mathrm{T}}\xi, \boldsymbol{a}\rangle_{\mathbb{R}^3}.$$

Take the explicit expressions

$$\boldsymbol{F}_n := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & \frac{1}{n} \end{pmatrix}, \quad \xi = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \|\boldsymbol{F}_n^{\mathrm{T}}\xi\|^2 = \frac{1}{n^2}, \quad \boldsymbol{a} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \eta = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}.$$

This leads to

$$\langle \boldsymbol{F}_n\boldsymbol{a}, \boldsymbol{F}_n\eta\rangle_{\mathbb{R}^3} = -1 + \frac{1}{3n^2}, \quad \langle \boldsymbol{a}, \eta\rangle_{\mathbb{R}^3} = \frac{1}{3}$$

and altogether we have for some reasonable $n$

$$D_F^2(\|\boldsymbol{F}_n^{\mathrm{T}}\boldsymbol{F}_n\boldsymbol{a}\|_{\mathbb{R}^3}^2).(\xi \otimes \eta, \xi \otimes \eta) \leqslant \left(-2 + \frac{2}{3n^2}\right)\frac{1}{3} + \frac{4}{n} < 0.$$

Observe, that the isotropic counterpart $\mathrm{tr}[\boldsymbol{C}^2] = \|\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}\|^2$ is a convex function of $\boldsymbol{F}$ (see Proof (1)). □

Up to now we can conclude that we cannot use the invariant $J_5$ and the polynomial invariant $I_1J_4$ as single terms for the construction of a free energy term. To take into account quadratic expressions of these terms within the ansatz functions we remember that $\mathrm{Cof}[\boldsymbol{C}]$ is a quadratic function in the right Cauchy–Green tensor. Furthermore, it seems reasonable from a physical point of view to construct a polynomial mixed invariant, which reflects the deformation of a preferred area element of an infinitesimal volume of the considered body. With this geometric motivation we start with the characteristic polynomial of the matrix $\boldsymbol{C}$ (see the Cayley-Hamilton Theorem A.8). Multiplication of the characteristic polynomial with $\boldsymbol{C}^{-1}\boldsymbol{M}$ yields with $\mathrm{Cof}\,\boldsymbol{C} = \mathrm{Adj}\,\boldsymbol{C}$

$$\boldsymbol{C}^2\boldsymbol{M} - I_1\boldsymbol{C}\boldsymbol{M} + I_2\boldsymbol{M} - \mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M} = \boldsymbol{0}. \tag{3.45}$$

Taking the trace of the Eq. (3.45) leads with the abbreviations (3.16) and (3.19) to the expression

$$K_1 := \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M}] = J_5 - I_1J_4 + I_2\bar{I}_M, \tag{3.46}$$

which is a polyconvex polynomial function in the non-polyconvex individual terms $J_5$ and $J_4I_1$. The proof of the convexity of the powers of $K_1$ is straightforward by replacing $\boldsymbol{F}$ with $\mathrm{Cof}\boldsymbol{F}$ in Proof (4). Thus $K_1$ represents a quadratic and polyconvex expression in $\boldsymbol{C}$ which replaces the non-elliptic term $J_5$. Based on the definition (3.46 first part) of $K_1$ we can give a rather simple geometric interpretation of this polynomial invariant. Starting from

$$K_1 = \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M}] = \mathrm{Cof}[\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}] : \boldsymbol{a} \otimes \boldsymbol{a} = (\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a})(\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}) = \|\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}\|^2, \tag{3.47}$$

we see that $\sqrt{K_1} = \|\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}\|$ controls the deformation of the area element with unit normal $\boldsymbol{a}$. Consider the deformation of a unit cube with $\boldsymbol{F} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ where $\lambda_3$ represents the stretch in preferred direction, then we arrive at $\sqrt{K_1} = \lambda_1\lambda_2$. An illustration of this simple example is given in Fig. 3a where $\lambda_1\lambda_2$ is represented by the shaded area.

Let us now specify some representative polyconvex functions in the invariants $K_1$ and $I_3$:

$$\psi_{22} := \gamma_1 K_1, \quad \psi_{23} := \gamma_2 K_1^2, \quad \psi_{24} := \gamma_5 K_1^3, \\ \psi_{25} := \gamma_3\frac{K_1}{I_3^{1/3}}, \quad \psi_{26} := \gamma_6\frac{K_1^2}{I_3^{2/3}} \tag{3.48}$$

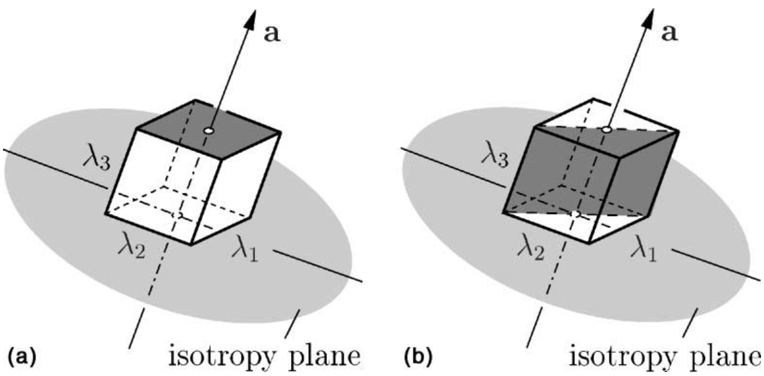


Fig. 3. Geometric interpretation of the the polynomial invariants: (a) $K_1$ and (b) $K_3$.

with $\gamma_i > 0$. It should be noted that $K_1/I_3^{1/3}$ and $K_1^2/I_3^{2/3}$ are coupled volumetric–isochoric terms. In Proof (4) we have seen that powers of $\mathrm{tr}[\boldsymbol{CM}]$ are polyconvex; these functions represent powers of the stretch in the preferred direction. As such it seems to be elemental that stretches in the isotropy plane also make sense as specific ansatz functions. For the construction of such further mixed terms we use the redundant structural tensor (3.25). We obtain the polynomial invariant

$$K_2 := \mathrm{tr}[\boldsymbol{CD}] = I_1 - J_4, \tag{3.49}$$

which represents the square stretch in the isotropy plane relative to the undeformed state. Of course, it is not necessary to introduce this *redundant* tensorial quantity with regard to the polynomial basis, but for the analysis of the convexity properties it is helpful. With the relation

$$K_2^k = (\mathrm{tr}[\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}(\boldsymbol{1} - \boldsymbol{M})])^k = (\|\boldsymbol{F}\|^2 - \|\boldsymbol{Fa}\|^2_{\mathbb{R}^3})^k, \tag{3.50}$$

we may apply the same reasoning as in Proof (4). Observe that

$$(\|\boldsymbol{F}\|^2 - \|\boldsymbol{Fa}\|^2_{\mathbb{R}^3}) \geqslant 0 \quad \text{if } \|\boldsymbol{a}\|_{\mathbb{R}^3} = 1$$

(see also the discussion in the Appendix Lemma C.2). With the same physical motivations as used for the construction of $K_1$ and $K_2$ we are now looking for a polynomial invariant which controls the area elements of an infinitesimal volume, characterized by normals lying in the isotropy plane. Using $\mathrm{Cof}\boldsymbol{F}$ instead of $\boldsymbol{F}$ in (3.50) we obtain for the exponent $k = 1$ the expression

$$K_3 := \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{D}] = I_1J_4 - J_5 + I_1(1 - \bar{I}_M) = I_1J_4 - J_5. \tag{3.51}$$

As $K_1$, $K_3$ represents a quadratic and polyconvex expression in $\boldsymbol{C}$. In an analogous way to the geometric interpretation of $K_1$ we can interpret the polynomial invariant $K_3$. After some algebraic manipulations of (3.51) we obtain

$$K_3 = \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{D}] = \|\mathrm{Cof}[\boldsymbol{F}]\|^2 - \|\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}\|^2, \tag{3.52}$$

we see that $\sqrt{K_3}$ controls the deformation of an area element with a normal in the isotropy plane, i.e. with a normal perpendicular to $\boldsymbol{a}$. Consider again the deformation of a unit cube with $\boldsymbol{F} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ with $\lambda_3$ being the stretch in the preferred direction. Thus $\lambda_1, \lambda_2$ present the stretches of the edges of the unit cube in the isotropy plane and we arrive at $\sqrt{K_3} = \lambda_3(\lambda_2^2 + \lambda_1^2)^{1/2}$. An illustration of this is given in Fig. 3b; the area element $\lambda_3(\lambda_2^2 + \lambda_1^2)^{1/2}$ controlled by $K_3$ is shaded. Some possible polyconvex functions in $K_2$, $K_3$ and $I_3$ are listed in (3.53)

$$\psi_{27} := \phi_1 K_2, \quad \psi_{28} := \phi_2 K_2^2, \quad \psi_{29} := \phi_3 K_3, \quad \psi_{30} := \phi_4 K_3^2,$$
$$\psi_{31} := \phi_5 \frac{K_2}{I_3^{1/3}}, \quad \psi_{32} := \phi_6 \frac{K_3}{I_3^{1/3}}, \quad \psi_{33} := \phi_7 \frac{K_2^2}{I_3^{2/3}}, \quad \psi_{34} := \phi_8 \frac{K_3^2}{I_3^{1/3}} \tag{3.53}$$

with $\phi_i > 0$. For the proof of the polyconvexity of $\psi_i, i = 31, \ldots, 34$ see Lemma C.3. Before considering further, more complicated, functions we give a physical interpretation of the terms in $K_1/I_3^{1/3}$ and $K_3/I_3^{1/3}$. As a simple example we consider a process with $\det \boldsymbol{F} = 1$ which is constant over the considered domain. The isochoric part of the deformation of the cylinder shown in Fig. 4 is given by $\widetilde{\boldsymbol{F}} = \mathrm{diag}(\lambda^{2/3}, \lambda^{-1/3}, \lambda^{-1/3})$; let

$$\psi_{\mathrm{iso}} := c^+ \|\mathrm{Cof}\,\widetilde{\boldsymbol{F}}\|^2 = c^+(\lambda^{-4/3} + 2\lambda^{2/3})$$

be one part of the associated isotropic free energy. On the other hand we consider an anisotropic energy term of the form $\psi_a := c_1^+ K_1/I_3^{1/3} + c_2^+ K_3/I_3^{1/3}$. For the assumed isochoric process $\psi_a$ can be rewritten as

$$\psi_a = c_1^+ \|\mathrm{Cof}\,\widetilde{\boldsymbol{F}}\boldsymbol{a}\|^2 + c_2^+(\|\mathrm{Cof}\,\widetilde{\boldsymbol{F}}\|^2 - \|\mathrm{Cof}\,\widetilde{\boldsymbol{F}}\boldsymbol{a}\|^2) = c_1^+ \lambda^{-4/3} + 2c_2^+ \lambda^{2/3}.$$

This equation states that the energy associated with the isochoric deformation can be weighted with respect to the deformation of the area elements characterized by normals in preferred direction and within the isotropy plane. So in general it should be possible to obtain at least one energetic equivalent isochoric deformation which differs from the one in Fig. 4a. Set e.g. $c_2^+ = \alpha c^+$ and $c_1^+ = f(\alpha)c^+$ with $\alpha, f(\alpha) \in \mathbb{R}_+$. Then we arrive with the condition of equivalence of the energetic terms $\psi_{\mathrm{iso}} = \psi_a$ at

$$f(\alpha) = 1 + 2\bar{\lambda}^2(1 - \alpha),$$

with $\alpha \in (0, 1)$. Here $\bar{\lambda}$ characterizes a fixed value of the deformation for which the energetic equivalence is postulated, thus it is no variable. A visualization of such an equivalent configuration is depicted in Fig. 4b. For $\alpha = 1$ the parameters are $c^+ = c_1^+ = c_2^+$ and we arrive at the isochoric representation.

Examples for further polynomial invariants in elements of the polynomial basis $\mathscr{P}_1$ are listed in (3.59). As shown in Proof 3, the term $J_4 I_1 = \mathrm{tr}[\boldsymbol{MC}]\mathrm{tr}\boldsymbol{C}$ is not elliptic and hence not polyconvex. Let us now consider an ansatz function of the form

$$\boldsymbol{F} \mapsto \|\boldsymbol{F}\|^4 + \|\boldsymbol{F}\|^2 \|\boldsymbol{F}\boldsymbol{a}\|^2 = I_1^2 + I_1 J_4, \tag{3.54}$$

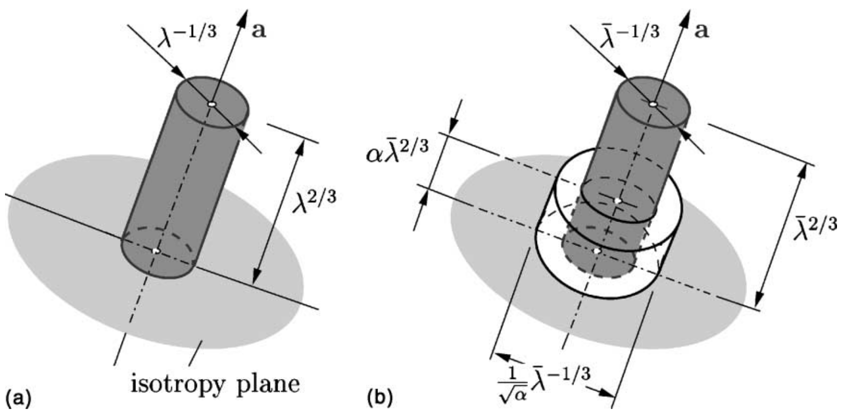


Fig. 4. Interpretation of the polynomial invariants $K_1/I_3^{1/3}$ and $K_3/I_3^{1/3}$ for an assumed isochoric deformation process. Picture (a) shows the isochoric deformation of the uniaxial stretched cylinder of Fig. 2 and Picture (b) represents an energetic weighting of the parts controlled by $K_1/I_3^{1/3}$ and $K_3/I_3^{1/3}$.

which is convex in $\boldsymbol{F}$. The proof of this is given in Lemma C.2, Eq. 4. Replacing $\boldsymbol{F}$ with $\mathrm{Cof}\boldsymbol{F}$ yields yet other polyconvex functions, so we obtain

$$\left.\begin{array}{l}\psi_{35} := \kappa_1\{(\mathrm{tr}\boldsymbol{C})^2 + \mathrm{tr}[\boldsymbol{MC}]\mathrm{tr}\boldsymbol{C}\} \\ \psi_{36} := \kappa_2\{(\mathrm{tr}\,\mathrm{Cof}\boldsymbol{C})^2 + \mathrm{tr}[\boldsymbol{M}\mathrm{Cof}\boldsymbol{C}]\mathrm{tr}\,\mathrm{Cof}\boldsymbol{C}\}\end{array}\right\}. \tag{3.55}$$

It should be noted that $\mathrm{tr}[\boldsymbol{M}\mathrm{Cof}\boldsymbol{C}]\mathrm{tr}\,\mathrm{Cof}\boldsymbol{C}$ alone is also not elliptic. In an analogous way we can construct polyconvex functions which include the non-elliptic terms $\mathrm{tr}[\boldsymbol{DC}]\mathrm{tr}\boldsymbol{C}$ and $\mathrm{tr}[\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}]\mathrm{tr}\,\mathrm{Cof}\boldsymbol{C}$. Consider the convex mapping

$$\boldsymbol{F} \mapsto 2\|\boldsymbol{F}\|^4 + \|\boldsymbol{F}\|^2\|\boldsymbol{F}(\mathbf{1} - \boldsymbol{M})\|^2, \tag{3.56}$$

or alternatively in $\mathrm{Cof}\boldsymbol{F}$ instead of $\boldsymbol{F}$. For the proof, see Lemma C.2, Eq. 5. Thus we obtain

$$\left.\begin{array}{l}\psi_{37} := \kappa_4\{2(\mathrm{tr}\boldsymbol{C})^2 + \mathrm{tr}[\boldsymbol{DC}]\mathrm{tr}\boldsymbol{C}\} \\ \psi_{38} := \kappa_5\{2(\mathrm{tr}\,\mathrm{Cof}\boldsymbol{C})^2 + \mathrm{tr}[\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}]\mathrm{tr}\,\mathrm{Cof}\boldsymbol{C}\}\end{array}\right\}. \tag{3.57}$$

On the other hand the difference of some polyconvex functions could be of interest in order to get further ansatz functions. For this reason let us define the free energy terms

$$\left.\begin{array}{l}\psi_{39} := \kappa_6\{a_1^+(\mathrm{tr}\boldsymbol{C}) - b_1^+(\mathrm{tr}[\boldsymbol{MC}])\} \\ \psi_{40} := \kappa_7\{a_2^+(\mathrm{tr}\,\mathrm{Cof}\boldsymbol{C}) - b_2^+(\mathrm{tr}[\boldsymbol{M}\mathrm{Cof}\boldsymbol{C}])\}\end{array}\right\} \quad \text{with} \quad \left\{\begin{array}{l}a_1^+ \geqslant b_1^+ \\ a_2^+ \geqslant b_2^+\end{array}\right., \tag{3.58}$$

with the positive constants $a_i^+$, $b_i^+$, $i = 1, 2$. The convexity of these equations with respect to $\boldsymbol{F}$ and $\mathrm{Cof}\boldsymbol{F}$ is obvious, due to the convexity of $\mathrm{tr}[\boldsymbol{CD}] = \mathrm{tr}\boldsymbol{C} - \mathrm{tr}[\boldsymbol{CM}]$ and $\mathrm{tr}[\mathrm{Cof}\boldsymbol{CD}] = \mathrm{tr}\,\mathrm{Cof}\boldsymbol{C} - \mathrm{tr}[\boldsymbol{M}\mathrm{Cof}\boldsymbol{C}]$. The expressions of the functions $\psi_i, i = 35, \ldots, 40$ in the elements of the polynomial basis $\mathscr{P}_1$ are given in (3.59), where we have chosen the constants $a_1^+ = 3$, $b_1^+ = 2$, $a_2^+ = 3$, $b_2^+ = 2$.

$$\begin{array}{ll}\psi_{35} := \kappa_1(I_1^2 + J_4I_1), & \psi_{36} := \kappa_2(2I_2^2 + I_2J_5 - I_1I_2J_4) \\ \psi_{37} := \kappa_4(3I_1^2 - I_1J_4), & \psi_{38} := \kappa_5(2I_2^2 + I_1I_2J_4 - I_2J_5) \\ \psi_{39} := \kappa_6(3I_1 - 2J_4), & \psi_{40} := \kappa_7(I_2 - 2J_5 + 2I_1J_4)\end{array} \tag{3.59}$$

with $\kappa_i > 0$. The proof of the convexity condition for the individual terms is given in the Appendix (see Lemma C.2). Examples of generic anisotropic exponential polyconvex functions are given in Appendix C, Lemma C.4. In this context see also the examples of some representative non-elliptic functions in Appendix C, Lemmas C.8 and C.9. With the variety of polyconvex, isotropic and transversely isotropic free energy functions derived above, it should be possible to model a wide range of different physical stress–strain relations. The stresses appear with (3.40) in the form

$$\boldsymbol{S} := \boldsymbol{S}_1 + 2\sum_{j=1}^{n}\left\{\frac{\partial\psi_j}{\partial J_4}\boldsymbol{M} + \frac{\partial\psi_j}{\partial J_5}(\boldsymbol{CM} + \boldsymbol{MC})\right\}. \tag{3.60}$$

The material tangent moduli $\mathbb{C}$ appear with (3.41) in index-representation in the form

$$\begin{aligned}\mathbb{C}^{ABCD} = \mathbb{C}_1^{ABCD} + 4\sum_{j=1}^{n}\Bigg[ & \frac{\partial^2\psi_j}{\partial J_4\,\partial J_4}\boldsymbol{M}^{AB}\boldsymbol{M}^{CD} + \frac{\partial^2\psi_j}{\partial J_5\,\partial J_5}\{\boldsymbol{CM}+\boldsymbol{MC}\}^{AB}\{\boldsymbol{CM}+\boldsymbol{MC}\}^{CD} \\ & + \frac{\partial^2\psi_j}{\partial I_1\,\partial J_4}[\boldsymbol{G}^{AB}\boldsymbol{M}^{CD}+\boldsymbol{M}^{AB}\boldsymbol{G}^{CD}] + \frac{\partial^2\psi_j}{\partial I_1\,\partial J_5}[\boldsymbol{G}^{AB}\{\boldsymbol{CM}+\boldsymbol{MC}\}^{CD}+\{\boldsymbol{CM}+\boldsymbol{MC}\}^{AB}\boldsymbol{G}^{CD}] \\ & + \frac{\partial^2\psi_j}{\partial I_2\,\partial J_4}[\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{AB}\boldsymbol{M}^{CD}+\boldsymbol{M}^{AB}\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{CD}] + \frac{\partial^2\psi_j}{\partial I_2\,\partial J_5}[\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{AB}\{\boldsymbol{CM}+\boldsymbol{MC}\}^{CD} \\ & + \{\boldsymbol{CM}+\boldsymbol{MC}\}^{AB}\{I_1\boldsymbol{G}-\boldsymbol{C}\}^{CD}] + \frac{\partial^2\psi_j}{\partial I_3\,\partial J_4}[\{\mathrm{Cof}\,\boldsymbol{C}\}^{AB}\boldsymbol{M}^{CD}+\boldsymbol{M}^{AB}\{\mathrm{Cof}\,\boldsymbol{C}\}^{CD}] \\ & + \frac{\partial^2\psi_j}{\partial I_3\,\partial J_5}[\{\mathrm{Cof}\,\boldsymbol{C}\}^{AB}\{\boldsymbol{CM}+\boldsymbol{MC}\}^{CD}+\{\boldsymbol{CM}+\boldsymbol{MC}\}^{AB}\{\mathrm{Cof}\,\boldsymbol{C}\}^{CD}] \\ & + \frac{\partial^2\psi_j}{\partial J_4\,\partial J_5}[\{\boldsymbol{CM}+\boldsymbol{MC}\}^{AB}\boldsymbol{M}^{CD}+\boldsymbol{M}^{AB}\{\boldsymbol{CM}+\boldsymbol{MC}\}^{CD}] + \frac{\partial\psi_j}{\partial J_5}[\boldsymbol{G}^{AC}\boldsymbol{M}^{BD}+\boldsymbol{M}^{AC}\boldsymbol{G}^{BD}]\Bigg].\end{aligned} \tag{3.61}$$

Here terms like $(\bullet)^{AB}$ characterize the contravariant index representations of the individual tensor expressions, e.g. $\{\boldsymbol{CM}+\boldsymbol{MC}\}^{AB}$ denotes $G^{AC}C_{CD}M^{DB}+M^{AC}C_{CD}G^{DB}$.

### *3.3. Spatial formulation*

For isotropic material response the Kirchhoff stresses $\boldsymbol{\tau}$ can be derived directly by the derivative of the free energy function with respect to the Finger tensor $\boldsymbol{b} := \boldsymbol{F}\boldsymbol{F}^{\mathrm{T}}$ (see e.g. Miehe, 1994). For the anisotropic case the Kirchhoff stresses and associated spatial moduli $\mathbb{c}$ can be computed via a push-forward operation of the second Piola–Kirchhoff stresses $\boldsymbol{S}$ and the associated moduli $\mathbb{C}$, i.e.

$$\tau^{ab} := F^a_A F^b_B S^{AB} \quad \text{and} \quad \mathbb{c}^{abcd} := F^a_A F^b_B F^c_C F^d_D \mathbb{C}^{ABCD}, \tag{3.62}$$

or by a direct evaluation of the Doyle Ericksen formula (2.6 second part). Regarding $\boldsymbol{C}$ as a function of the point values of the deformation gradient $\boldsymbol{F}$ and the spatial metric $\boldsymbol{g}$, we are left with $\boldsymbol{C}=\widehat{\boldsymbol{C}}(\boldsymbol{F},\boldsymbol{g})$ (see Marsden and Hughes, 1983). The only modification of the stress functions (3.60) in combination with (3.40) is referred to the tensor generators, because the derivatives of the free energy function with respect to the invariants remain unchanged. Thus we only need the derivatives of the invariants with respect to the covariant metric coefficients, e.g. we obtain for

$$\frac{\partial I_1}{\partial g_{ab}} = \frac{\partial(F^c_A F^d_B g_{cd} G^{AB})}{\partial g_{ab}} = F^a_A F^b_B G^{AB} := b^{ab},$$

which is the index representation of the Finger tensor $\boldsymbol{b}$. In an analogous way we get the derivatives of the other invariants. In direct notation we obtain the expressions

$$\left.\begin{aligned} \frac{\partial I_1}{\partial \boldsymbol{g}} &= \frac{\partial \mathrm{tr}[\widehat{\boldsymbol{C}}(\boldsymbol{F},\boldsymbol{g})]}{\partial \boldsymbol{g}} = \boldsymbol{b} \\ \frac{\partial I_2}{\partial \boldsymbol{g}} &= \frac{\partial (I_1^2 - J_2)/2}{\partial \boldsymbol{g}} = I_1\boldsymbol{b} - \frac{1}{2}\frac{\partial \mathrm{tr}[(\widehat{\boldsymbol{C}}(\boldsymbol{F},\boldsymbol{g}))^2]}{\partial \boldsymbol{g}} = I_1\boldsymbol{b} - \boldsymbol{b}^2 \\ \frac{\partial I_3}{\partial \boldsymbol{g}} &= \frac{\partial I_3}{\partial \boldsymbol{C}} : \frac{\partial \widehat{\boldsymbol{C}}(\boldsymbol{F},\boldsymbol{g})}{\partial \boldsymbol{g}} = I_3\boldsymbol{g}^{-1} \\ \frac{\partial J_4}{\partial \boldsymbol{g}} &= \frac{\partial(\widehat{\boldsymbol{C}}(\boldsymbol{F},\boldsymbol{g})) : \boldsymbol{M}}{\partial \boldsymbol{g}} = \tilde{\boldsymbol{a}} \otimes \tilde{\boldsymbol{a}} \\ \frac{\partial J_5}{\partial \boldsymbol{g}} &= \frac{\partial \mathrm{tr}[(\widehat{\boldsymbol{C}}(\boldsymbol{F},\boldsymbol{g}))^2\boldsymbol{M}]}{\partial \boldsymbol{g}} = \boldsymbol{b}\tilde{\boldsymbol{a}} \otimes \boldsymbol{b}\tilde{\boldsymbol{a}} \end{aligned}\right\}. \tag{3.63}$$

In this direct representation we have dropped the obvious dependence of the quantities with respect to the metric tensors. Finally the Kirchhoff stresses appear in the form

$$\boldsymbol{\tau} := 2\sum_{j=1}^{n}\left[\left(\frac{\partial\psi_j}{\partial I_1}+\frac{\partial\psi_j}{\partial I_2}I_1\right)\boldsymbol{b}-\frac{\partial\psi_j}{\partial I_2}\boldsymbol{b}^2+\frac{\partial\psi_j}{\partial I_3}I_3\boldsymbol{g}^{-1}+\frac{\partial\psi_j}{\partial J_4}\tilde{\boldsymbol{a}}\otimes\tilde{\boldsymbol{a}}+\frac{\partial\psi_j}{\partial J_5}\boldsymbol{b}\tilde{\boldsymbol{a}}\otimes\boldsymbol{b}\tilde{\boldsymbol{a}}\right]. \tag{3.64}$$

The spatial moduli can be derived by $\mathbb{c} = 2\partial_g\boldsymbol{\tau}(\boldsymbol{C}(\boldsymbol{F},\boldsymbol{g}))$. For this derivation we have to take into account the intrinsic dependence of $\boldsymbol{b}^2$ with respect to $\boldsymbol{g}$, i.e. the index representation of the square of the Finger tensor is given by $b^{ac}g_{cd}b^{db}$. The computation of the spatial moduli is straightforward and therefore omitted here.

## 4. Stress free reference configuration and linearization

In this section we analyse the free energy functions with respect to the natural state condition, i.e. the stresses have to be zero in the reference configuration. Furthermore, we are interested in the linearized stress quantities near the reference configuration in order to identify moduli obtained by the invariant formulation with some well-known linear transversely isotropic moduli. The natural state is characterized by $\boldsymbol{F} = \boldsymbol{1}$ and the invariants have the values

$$I_1 = 3, \quad I_2 = 3, \quad I_3 = 1, \quad J_4 = J_5 = \bar{I}_M = \mathrm{tr}\boldsymbol{M} = 1. \tag{4.65}$$

Consequently the stress condition for the natural state, i.e. $\boldsymbol{S}(\boldsymbol{1}) = \boldsymbol{0}$, leads with (3.40) and (3.60) to the equation

$$2\sum_{j=1}^{n}\left\{\left(\frac{\partial\psi_j}{\partial I_1}+2\frac{\partial\psi_j}{\partial I_2}+\frac{\partial\psi_j}{\partial I_3}\right)\boldsymbol{1}+\left(\frac{\partial\psi_j}{\partial J_4}+2\frac{\partial\psi_j}{\partial J_5}\right)\boldsymbol{M}\right\} = \boldsymbol{0}. \tag{4.66}$$

The linearized moduli $\mathbb{C}_0$ at the reference configuration are obtained by linearization of the stress response functions (3.40) and (3.60). Thus we obtain with the Green–Lagrange strain tensor $\boldsymbol{E} := (1/2)(\boldsymbol{C}-\boldsymbol{1})$, the equation

$$\mathrm{Lin}[\boldsymbol{S}] = \boldsymbol{S}(\boldsymbol{1}) + \mathbb{C}_0 : \mathrm{Lin}[\boldsymbol{E}] \quad \text{with } \mathbb{C}_0 := 2\partial_C\boldsymbol{S}|_{\boldsymbol{1}} = 4\partial^2_C\psi|_{\boldsymbol{1}}. \tag{4.67}$$

The terms $\mathrm{Lin}[\boldsymbol{S}] =: \bar{\boldsymbol{\sigma}}$ present the linearized stress tensor and $\mathrm{Lin}[\boldsymbol{E}] =: \boldsymbol{\varepsilon}$ the linearized strain tensor in the reference configuration, respectively. The classical matrix notation of transverse isotropic material response in the case of small strains is given with the $X_3$-axis as axis of symmetry by the linear relationship

$$\begin{bmatrix}\bar{\sigma}_{11}\\ \bar{\sigma}_{22}\\ \bar{\sigma}_{33}\\ \bar{\sigma}_{12}\\ \bar{\sigma}_{23}\\ \bar{\sigma}_{13}\end{bmatrix} = \begin{bmatrix}\mathbb{C}_{11} & \mathbb{C}_{12} & \mathbb{C}_{13} & 0 & 0 & 0\\ \mathbb{C}_{12} & \mathbb{C}_{11} & \mathbb{C}_{13} & 0 & 0 & 0\\ \mathbb{C}_{13} & \mathbb{C}_{13} & \mathbb{C}_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & \frac{1}{2}(\mathbb{C}_{11}-\mathbb{C}_{12}) & 0 & 0\\ 0 & 0 & 0 & 0 & \mathbb{C}_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & \mathbb{C}_{44}\end{bmatrix}\begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ 2\varepsilon_{12}\\ 2\varepsilon_{23}\\ 2\varepsilon_{13}\end{bmatrix}. \tag{4.68}$$

From (4.67) it follows that the linearized moduli are obtained by evaluation of (3.61) at $\boldsymbol{C} = \boldsymbol{1}$. The linearization of (3.61) with (3.41) leads to

$$\begin{aligned}\mathbb{C}_0^{ABCD} = {}& c_1\boldsymbol{G}^{AB}\boldsymbol{G}^{CD} + c_2\{\boldsymbol{G}^{AB}\boldsymbol{G}^{CD} - \boldsymbol{G}^{AC}\boldsymbol{G}^{BD}\} + c_3\boldsymbol{M}^{AB}\boldsymbol{M}^{CD} + c_4[\boldsymbol{G}^{AB}\boldsymbol{M}^{CD} + \boldsymbol{M}^{AB}\boldsymbol{G}^{CD}]\\ & + c_5(\boldsymbol{G}^{AC}\boldsymbol{M}^{BD} + \boldsymbol{M}^{AC}\boldsymbol{G}^{BD})\end{aligned} \tag{4.69}$$

with the abbreviations

$$\left.\begin{aligned} c_1 &= 4\sum_{j=1}^{n}\left(\frac{\partial^2\psi_j}{\partial I_1\partial I_1}+4\frac{\partial^2\psi_j}{\partial I_2\partial I_2}+\frac{\partial^2\psi_j}{\partial I_3\partial I_3}+4\frac{\partial^2\psi_j}{\partial I_2\partial I_1}+2\frac{\partial^2\psi_j}{\partial I_3\partial I_1}+4\frac{\partial^2\psi_j}{\partial I_3\partial I_2}\right)\\ c_2 &= 4\sum_{j=1}^{n}\left(\frac{\partial\psi_j}{\partial I_2}+\frac{\partial\psi_j}{\partial I_3}\right)\\ c_3 &= 4\sum_{j=1}^{n}\left(\frac{\partial^2\psi_j}{\partial J_4\partial J_4}+4\frac{\partial^2\psi_j}{\partial J_5\partial J_5}+4\frac{\partial^2\psi_j}{\partial J_4\partial J_5}\right)\\ c_4 &= 4\sum_{j=1}^{n}\left(\frac{\partial^2\psi_j}{\partial I_1\partial J_4}+2\frac{\partial^2\psi_j}{\partial I_1\partial J_5}+2\frac{\partial^2\psi_j}{\partial I_2\partial J_4}+4\frac{\partial^2\psi_j}{\partial I_2\partial J_5}+\frac{\partial^2\psi_j}{\partial I_3\partial J_4}+2\frac{\partial^2\psi_j}{\partial I_3\partial J_5}\right)\\ c_5 &= 4\sum_{j=1}^{n}\frac{\partial\psi_j}{\partial J_5} \end{aligned}\right\}. \tag{4.70}$$

With the $X_3$-axis as the axis of symmetry we have $\boldsymbol{a} = (0,0,1)^{\mathrm{T}}$, $\boldsymbol{M} = \mathrm{diag}(0,0,1)$ and with the same index arrangement as in (4.68) we obtain from (4.69) the linearized moduli

$$\mathbb{C}_0 = \begin{bmatrix} c_1 & c_1+c_2 & c_1+c_2+c_4 & 0 & 0 & 0\\ c_1+c_2 & c_1 & c_1+c_2+c_4 & 0 & 0 & 0\\ c_1+c_2+c_4 & c_1+c_2+c_4 & c_1+c_3+2(c_4+c_5) & 0 & 0 & 0\\ 0 & 0 & 0 & \frac{-c_2}{2} & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{c_5-c_2}{2} & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{c_5-c_2}{2} \end{bmatrix}. \tag{4.71}$$

From Eq. (4.66) and the comparison of (4.71) with the matrix representation of the classical moduli (4.68) we obtain seven equations for the identification of the linearized moduli of the invariant formulation. This is consistent with the minimal number of ansatz functions for a quadratic free energy function introduced in (3.43). We need a minimum of five parameters (functions) to identify the individual moduli and two parameters (functions) to fulfill the condition of a stress-free reference configuration.

**Remark.** As a special case we obtain a family of Ogden-type materials for isotropic material response (see Ciarlet, 1988). We choose a compressible Mooney-Rivlin model of the form

$$\psi_{\mathrm{iso}} := \alpha_1\mathrm{tr}[\boldsymbol{C}] + \eta_1\mathrm{tr}[\mathrm{Cof}\,\boldsymbol{C}] + \delta_1 J^2 - \delta_2\ln(J), \tag{4.72}$$

with $J^2 = \det\boldsymbol{C}$. The two isotropic moduli near a natural state are characterized by

$$\mathbb{C}_{13} = \mathbb{C}_{12}, \quad \mathbb{C}_{33} = \mathbb{C}_{11}, \quad \mathbb{C}_{44} = \frac{1}{2}(\mathbb{C}_{11} - \mathbb{C}_{12}). \tag{4.73}$$

From the condition of a stress-free reference configuration (4.66) we obtain the equation

$$2\alpha_1 + 4\eta_1 + 2\delta_1 - \delta_2 = 0. \tag{4.74}$$

The relations between the Ogden-parameters and the isotropic moduli are

$$4\eta_1 + 4\delta_1 = \mathbb{C}_{12} \quad \text{and} \quad 2\delta_2 = \mathbb{C}_{11}. \tag{4.75}$$

The solution of the three equations (4.74) and (4.75) for the four material parameters $(\delta_1, \delta_2, \alpha_1, \eta_1) \in \mathbb{R}^+$ is

$$\left.\begin{array}{l}\alpha_1 := [\mathbb{C}_{11} + (\xi - 2)\mathbb{C}_{12}]/4 \\ \eta_1 := (1-\xi)\mathbb{C}_{12}/4 \\ \delta_1 := \xi\mathbb{C}_{12}/4 \\ \delta_2 := \mathbb{C}_{11}/2\end{array}\right\} \quad \text{with } \xi \in (0,1). \tag{4.76}$$

Let us introduce the expressions of the isotropic moduli in terms of the Lamé constants $\lambda$ and $\mu$, then we get $\mathbb{C}_{11} = \lambda + 2\mu$ and $\mathbb{C}_{12} = \lambda$. We see that it is always possible to choose a set of positive parameters for $\lambda > 0$ and $\mu > 0$ that satisfy (4.76) with $(\delta_1, \delta_2, \alpha_1, \eta_1) \in \mathbb{R}^+$ (see Ciarlet, 1988, pages 185–190). As a second example we consider a compressible Neo-Hookean model characterized by (4.72) with $\eta_1 = 0$. In this case we obtain the identification from (4.76) for $\xi = 1$, which means that we need a minimum of three material parameters in order to fulfill the above mentioned conditions.

## 5. Extension to orthotropic material response

In this section we discuss the construction of polyconvex orthotropic free-energy functions. Orthotropic materials are characterized by symmetry relations with respect to three orthogonal planes. The corresponding preferred directions are chosen as the intersections of these planes and are denoted by the vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ with unit length. Thus $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$ represents an orthonormal privileged frame. The material symmetry group is defined by

$$\mathscr{G}_o := \{\boldsymbol{I}; \boldsymbol{S}_1, \boldsymbol{S}_2, \boldsymbol{S}_3\}, \tag{5.77}$$

where $\boldsymbol{S}_1$, $\boldsymbol{S}_2$, $\boldsymbol{S}_3$ are the reflections with respect to the basis planes $(\boldsymbol{b}, \boldsymbol{c})$, $(\boldsymbol{c}, \boldsymbol{a})$ and $(\boldsymbol{a}, \boldsymbol{b})$, respectively. Based on this, we obtain for this symmetry group the structural tensors

$${}^1\boldsymbol{M} := \boldsymbol{a} \otimes \boldsymbol{a}, \quad {}^2\boldsymbol{M} := \boldsymbol{b} \otimes \boldsymbol{b} \quad \text{and} \quad {}^3\boldsymbol{M} := \boldsymbol{c} \otimes \boldsymbol{c}, \tag{5.78}$$

which represent the symmetry group (5.77). The structural tensors fulfill the conditions

$$\left.\begin{array}{l}{}^i\boldsymbol{M}^p = {}^i\boldsymbol{M}, \quad \operatorname{tr}{}^i\boldsymbol{M} = 1, \quad {}^i\boldsymbol{M}{}^j\boldsymbol{M} = 0 \quad \text{for } i \neq j,\ i,j = 1,2,3 \\ ({}^1\boldsymbol{M}\boldsymbol{C} + \boldsymbol{C}{}^1\boldsymbol{M}) + ({}^2\boldsymbol{M}\boldsymbol{C} + \boldsymbol{C}{}^2\boldsymbol{M}) + ({}^3\boldsymbol{M}\boldsymbol{C} + \boldsymbol{C}{}^3\boldsymbol{M}) = 2\boldsymbol{C} \\ \operatorname{tr}[{}^1\boldsymbol{M}\boldsymbol{C}] + \operatorname{tr}[{}^2\boldsymbol{M}\boldsymbol{C}] + \operatorname{tr}[{}^3\boldsymbol{M}\boldsymbol{C}] = \operatorname{tr}\boldsymbol{C}\end{array}\right\} \tag{5.79}$$

(see e.g. Boehler, 1987). Due to the fact that the sum of the three structural tensors yields $\sum_{i=1}^{3} {}^i\boldsymbol{M} = \boldsymbol{1}$ we may discard ${}^3\boldsymbol{M}$ from the set of structural tensors (5.78). So the integrity basis consists of

$$\mathscr{P}_3 := \{I_1, I_2, I_3, J_4, J_5, J_6, J_7; \bar{I}_{1M}, \bar{I}_{2M}\} \quad \text{or} \quad \mathscr{P}_4 := \{J_1, \dots, J_7; \bar{I}_{1M}, \bar{I}_{2M}\}. \tag{5.80}$$

The principal invariants $(I_1, I_2, I_3)$ and the basic invariants $(J_1, J_2, J_3)$ are defined in (3.16) and (3.17), respectively. The irreducible mixed invariants are given by

$$J_4 := \operatorname{tr}[{}^1\boldsymbol{M}\boldsymbol{C}] \quad J_5 := \operatorname{tr}[{}^1\boldsymbol{M}\boldsymbol{C}^2], \quad J_6 := \operatorname{tr}[{}^2\boldsymbol{M}\boldsymbol{C}], \quad J_7 := \operatorname{tr}[{}^2\boldsymbol{M}\boldsymbol{C}^2] \tag{5.81}$$

(see e.g. Spencer, 1971). Furthermore, the remaining trivial invariants are defined by $\bar{I}_{1M} := \operatorname{tr}{}^1\boldsymbol{M}$ and $\bar{I}_{2M} := \operatorname{tr}{}^2\boldsymbol{M}$. For the construction of the free energy function we assume the form

$$\psi = \sum_k \hat{\psi}_k(i_i | i_i \in \mathscr{P}_j) + c \quad \text{for } j = 3 \quad \text{or } j = 4, \tag{5.82}$$

where each function $\psi_k$ has to satisfy the polyconvexity condition a priori. All proposed polyconvex functions in the above sections in terms of $\boldsymbol{C}$ and $\boldsymbol{M}$ can be used by interchanging $\boldsymbol{M}$ with ${}^1\boldsymbol{M}$, ${}^2\boldsymbol{M}$ or ${}^3\boldsymbol{M}$. This holds also for the terms in $\boldsymbol{D}$; for this it seems advantageous to introduce the tensors ${}^i\boldsymbol{D} = \boldsymbol{1} - {}^i\boldsymbol{M}$ for $i = 1, 2, 3$. Based on this approach we obtain a variety of polyconvex functions in a straightforward manner, where the expressions in ${}^3\boldsymbol{M}$ and ${}^i\boldsymbol{D}$, $i = 1, 2, 3$ can easily be expressed as polynomial functions in terms of the elements of the integrity bases $\mathscr{P}_3$ or $\mathscr{P}_4$. The proofs of the polyconvexity of functions generated in this manner are already given above. Up to now we have only proposed individual polyconvex functions $\psi_k$ in terms of $(\boldsymbol{C}, {}^1\boldsymbol{M})$ or $(\boldsymbol{C}, {}^2\boldsymbol{M})$. For a general formulation we also need ansatz functions which include multiplicative terms in the mixed invariants with respect to different structural tensors. Often used terms in classical formulations, such as

$$J_4 J_6 = \mathrm{tr}[{}^1\boldsymbol{MC}]\mathrm{tr}[{}^2\boldsymbol{MC}] = \|\boldsymbol{Fa}\|^2\|\boldsymbol{Fb}\|^2, \tag{5.83}$$

are not polyconvex. The proof of the non-convexity of this term is straightforward (in this context see also Remark B.8, Appendix B). To overcome this problem we consider powers of linear convex combinations of positive polyconvex functions. Consider two convex functions $P_1(X, Y) \geqslant 0$ and $P_2(X, Y) \geqslant 0$, then functions of the form

$$P := [\lambda P_1(X, Y) + (1-\lambda)P_2(X, Y)]^q, \quad \lambda \in (0, 1) \quad \text{and} \quad q \in \mathbb{N}_+ \tag{5.84}$$

are polyconvex (see Corollary B.7). Thus we are able to construct a variety of free energy terms which involve multiplicative coupled terms in the mixed invariants associated to different structural tensors, e.g.

$$\left.\begin{array}{l} [\lambda \mathrm{tr}[{}^i\boldsymbol{MC}] + (1-\lambda)\mathrm{tr}[{}^j\boldsymbol{MC}]]^q \\ [\lambda \mathrm{tr}[{}^i\boldsymbol{MC}] + (1-\lambda)\mathrm{tr}[{}^j\boldsymbol{M}\mathrm{Cof}\boldsymbol{C}]]^q \end{array}\right\} \quad \text{with } \lambda \in (0, 1),\ i \neq j,\ q \in \mathbb{N}_+, \tag{5.85}$$

with $i, j = 1, 2, 3$. If we choose e.g. $q = 2$, then (5.85) first part leads with $i = 1$ and $j = 2$ to the invariant representation

$$\lambda^2 J_4^2 + 2\lambda(1-\lambda)J_4 J_6 + (1-\lambda)^2 J_6^2 \quad \text{with} \quad \lambda \in (0, 1), \tag{5.86}$$

which has a multiplicative term in the mixed invariants of the traces of the product of $(\boldsymbol{C}, {}^1\boldsymbol{M})$ and $(\boldsymbol{C}, {}^2\boldsymbol{M})$. Thus it is possible, in principal, to construct a wide variety of functions which are related in some sense to the classical formulations of orthotropic materials in the invariant setting.

## 6. Variational formulation and finite element discretization

In the following we give a brief summary of the corresponding boundary value problem and finite element formulation in the material description. Let $\mathscr{B}$ be the reference body of interest which is bounded by the surface $\partial\mathscr{B}$. The surface is partitioned into two disjointed parts $\partial\mathscr{B} = \partial\mathscr{B}_u \bigcup \partial\mathscr{B}_t$ with $\partial\mathscr{B}_u \bigcap \partial\mathscr{B}_t = \emptyset$. The equation of balance of linear momentum for the static case is governed by the first Piola-Krichhoff stresses $\boldsymbol{P} = \boldsymbol{FS}$ and the body force $\bar{\boldsymbol{f}}$ in the reference configuration

$$\mathrm{Div}[\boldsymbol{FS}] + \bar{\boldsymbol{f}} = \boldsymbol{0}. \tag{6.87}$$

The Dirichlet boundary conditions and the Neumann boundary conditions are given by

$$\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on } \partial\mathscr{B}_u \quad \text{and} \quad \boldsymbol{t} = \bar{\boldsymbol{t}} = \boldsymbol{PN} \quad \text{on } \partial\mathscr{B}_t, \tag{6.88}$$

respectively. Here $\boldsymbol{N}$ represents the unit exterior normal to the boundary surface $\partial\mathscr{B}_t$. With standard arguments of variational calculus we arrive at the variational problem

$$G(\boldsymbol{u}, \delta\boldsymbol{u}) = \int_{\mathscr{B}} \boldsymbol{S} : \delta\boldsymbol{E}\,\mathrm{d}V + G^{\mathrm{ext}} \quad \text{with } G^{\mathrm{ext}} := -\int_{\mathscr{B}} \bar{\boldsymbol{f}}\ \delta\boldsymbol{u}\,\mathrm{d}V - \int_{\partial\mathscr{B}_t} \bar{\boldsymbol{t}}\delta\boldsymbol{u}\,\mathrm{d}A, \tag{6.89}$$

where $\delta\boldsymbol{E} := \frac{1}{2}(\delta\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} + \boldsymbol{F}^{\mathrm{T}}\delta\boldsymbol{F})$ characterizes the virtual Green–Lagrangian strain tensor in terms of the virtual deformation gradient $\delta\boldsymbol{F} := \mathrm{Grad}\delta\boldsymbol{u}$. The equation of principle of virtual work (6.89) for a static equilibrium state of the considered body requires $G = 0$. For the solution of this non-linear equation we apply a standard Newton iteration scheme, which requires the consistent linearization of (6.89) in order to guarantee the quadratic convergence rate near the solution. Since the stress tensor $\boldsymbol{S}$ is symmetric, the linear increment of $G$ denoted by $\Delta G^{\text{ext}}$ is given by

$$\Delta G(\boldsymbol{u}, \delta\boldsymbol{u}, \Delta\boldsymbol{u}) := \int_{\mathscr{B}} (\delta\boldsymbol{E} : \mathbb{C} : \Delta\boldsymbol{E} + \delta\boldsymbol{F}\boldsymbol{S}\Delta\boldsymbol{F}^{\mathrm{T}})\, \mathrm{d}V, \tag{6.90}$$

where $\Delta\boldsymbol{E} := \frac{1}{2}(\Delta\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} + \boldsymbol{F}^{\mathrm{T}}\Delta\boldsymbol{F})$ denotes the incremental Green–Lagrange strain tensor as a function of the incremental deformation gradient $\Delta\boldsymbol{F} := \mathrm{Grad}\Delta\boldsymbol{u}$. The spatial discretization of the considered body $\mathscr{B} \approx \bigcup_{e=1}^{n_{\text{ele}}} \mathscr{B}^e$ with $n_{\text{ele}}$ finite elements $\mathscr{B}^e$ leads within a standard displacement approximation $\boldsymbol{u} = \sum_{I=1}^{\text{nel}} N^I \boldsymbol{d}_I$, $\delta\boldsymbol{u} = \sum_{I=1}^{\text{nel}} N^I \delta\boldsymbol{d}_I$, and $\Delta\boldsymbol{u} = \sum_{I=1}^{\text{nel}} N^I \Delta\boldsymbol{d}_I$, of the actual-, virtual-, and incremental-displacement fields, respectively, to a set of algebraic equations of the form which can be solved for the solution point $\boldsymbol{d}$. For a detailed discussion of this point we refer to the standard text books (Zienkiewicz and Taylor, 2000, Hughes, 1987 and others).

## 7. Numerical examples

In this section we analyse a three-dimensional tapered cantilever and a two-dimensional perforated plate with centered hole. In the first example we point out the influence of the anisotropy and in the second example we discuss the influence of the orientation of the preferred direction and compare the results for two sets of material parameters. The corresponding linearized moduli at the reference configuration are given for both material sets within the invariant formulation and in the classical notation.

### *7.1. 3D-analysis of a tapered cantilever*

In this example we consider a tapered cantilever clamped on the left hand side and subjected to a shearing deformation $\lambda\boldsymbol{F}$ in vertical direction with $\|\boldsymbol{F}\| = 1$ on the right hand side. Here $\lambda$ denotes the load parameter. The system and the boundary conditions are depicted in Fig. 5a and b shows the reference configuration, discretized with $20 \times 20 \times 5$ eight-noded standard displacement elements in horizontal, vertical and thickness direction. The thickness of the specimen is set to 1.

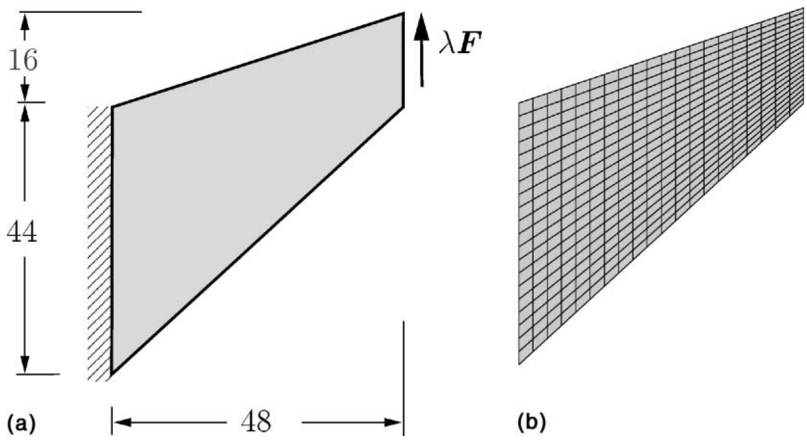


Fig. 5. Tapered Cantilever. (a) System and boundary conditions; (b) discretization with $20 \times 20 \times 5 = 2000$ eight-noded brick elements.

The chosen free energy function $\psi$ consists of seven additive terms $\tilde{\psi}_j$, in detail

$$\psi = \sum_{j=1}^{7} \tilde{\psi}_j(I_1, I_2, I_3, J_4, J_5) \quad \text{with } \tilde{\psi}_j | j = 1, \ldots, 7 = \psi_i | i = 1, 13, 19, 25, 30, 31, 33, \tag{7.91}$$

respectively. The number of ansatz functions is consistent with the treatment of the compressible Neo-Hookean material in the isotropic case, which requires three terms, see the end of the remark in Section 4. In this context see also the interpretation of Eq. (3.43). It should be noted that the function

$$\tilde{\psi}_1(I_1) = \alpha_1 \operatorname{tr}\boldsymbol{C} \tag{7.92}$$

is linear in the invariant $I_1$. As such it only effects the Second Piola–Kirchhoff stresses, i.e. $\tilde{\psi}_1(I_1)$ leads to a positive volumetric stress contribution. An anisotropic counterpart is $\psi_{16}(J_4)$; this linear term in $J_4$ leads to an anisotropic stress contribution with respect to the tensor generator $\boldsymbol{M}$. The remaining parts are

$$\left.\begin{array}{l} \tilde{\psi}_2(I_3) = \delta_5 1/\det\boldsymbol{C} \\ \tilde{\psi}_3(J_4) = \beta_2(\operatorname{tr}[\boldsymbol{MC}])^2 \\ \tilde{\psi}_4(I_1, I_2, I_3, J_4, J_5) = \gamma_3 \operatorname{tr}[\boldsymbol{M}\operatorname{Cof}\boldsymbol{C}]/(\det\boldsymbol{C})^{1/3} \\ \tilde{\psi}_5(I_1, J_4, J_5) = \phi_4(\operatorname{tr}[\boldsymbol{D}\operatorname{Cof}\boldsymbol{C}])^2 \\ \tilde{\psi}_6(I_1, I_3, J_4, J_5) = \phi_5 \operatorname{tr}[\boldsymbol{DC}]/(\det\boldsymbol{C})^{1/3} \\ \tilde{\psi}_7(I_1, I_3, J_4, J_5) = \phi_7(\operatorname{tr}[\boldsymbol{DC}])^2/(\det\boldsymbol{C})^{1/3} \end{array}\right\}. \tag{7.93}$$

With these ansatz functions we obtain from (4.66) the explicit expression

$$\left(2\alpha_1 + \frac{4}{3}\gamma_3 + 8\phi_4 + \frac{2}{3}\phi_5 + \frac{16}{3}\phi_7 - 2\delta_5\right)\boldsymbol{1} + (4\beta_2 - 2\gamma_3 + 8\phi_4 - 2\phi_5 - 8\phi_7)\boldsymbol{M} = \boldsymbol{0}, \tag{7.94}$$

for the vanishing stresses in the reference configuration. The coefficients of the linearized moduli (4.70) are given by

$$\left.\begin{array}{l} c_1 = 8\phi_4 + \frac{40}{9}\phi_7 + 8\delta_5 - \frac{8}{9}\gamma_3 + \frac{8}{9}\phi_5 \\ c_2 = \frac{8}{3}\gamma_3 - 4\delta_5 - \frac{8}{3}\phi_5 - \frac{16}{3}\phi_7 \\ c_3 = 8\beta_2 + 8\phi_4 + 8\phi_7 \\ c_4 = -\frac{8}{3}\gamma_3 + 24\phi_4 - \frac{8}{3}\phi_7 + \frac{4}{3}\phi_5 \\ c_5 = 4\gamma_3 - 16\phi_4 \end{array}\right\}. \tag{7.95}$$

The chosen material parameters of the polyconvex free energy function in the invariant setting are

$$\left.\begin{array}{llll} \alpha_1 = 2.6875, & \delta_5 = 136.41, & \beta_2 = 112.21, & \gamma_3 = 80.393 \\ \phi_4 = 5.7233, & \phi_5 = 162.15, & \phi_7 = 1.1920 & \end{array}\right\}. \tag{7.96}$$

The free energy function (7.91) with the parameters (7.96) will be referred to as material parameter set 1 (**MS 1**) in the following example.

Let the $X_3$-axis be the preferred direction; then the corresponding linearized moduli are

$$\mathbb{C}_{11} \approx 1215.0, \quad \mathbb{C}_{12} \approx 445.0, \quad \mathbb{C}_{13} \approx 581.0, \quad \mathbb{C}_{33} \approx 2900.0, \quad \mathbb{C}_{44} \approx 500.0. \tag{7.97}$$

The two-dimensional version of this test in the linear elastic range is often referred to as the Cook's membrane problem. It is a standard test for bending-dominated problems. In the isotropic case the deformed structure would be dominated by in-plane deformations. Here we are interested in the influence of the anisotropic constitutive laws. For the simulation the preferred direction was set to $\boldsymbol{a} = (1,1,1)^{\mathrm{T}}/\sqrt{3}$ and

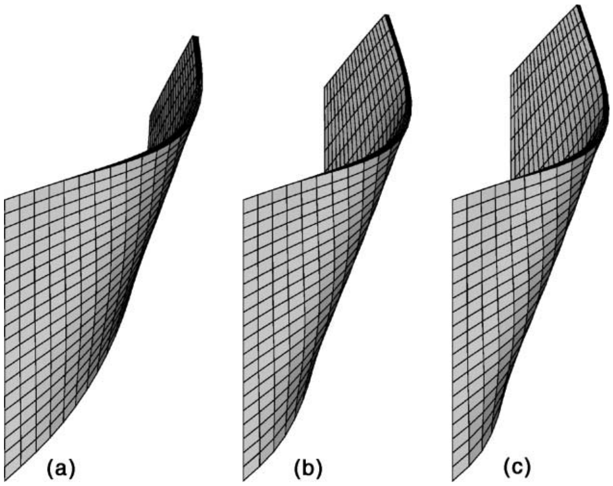


Fig. 6. Tapered Cantilever. Deformed configurations for selected load levels: (a) at $\lambda = 130$, (b) at $\lambda = 270$ and (c) at $\lambda = 400$.

the load parameter is increased by increments $\Delta\lambda = 1$ until a final value of $\lambda = 400$ is reached. Fig. 6a–c depicts the deformed structures of the beam at $\lambda = 130$, $\lambda = 270$ and $\lambda = 400$, respectively. In contrast to an isotropic material the anisotropic one leads to a salient out-of-plane bending deformation. This enormous out-of-plane bending is of course initiated by the orientation of the preferred direction.

### *7.2. Perforated plate with centered hole*

In this example we consider a rectangular plate with a centered hole with two different free energy functions and three different orientations for each. The preferred directions are assumed to be in the plane of the plate. The dimensions of the specimen are given in Fig. 7 and the thickness is set to $t = 1$.

The system is subjected to tension in horizontal direction. The left and right boundaries are pulled up to a final length of the specimen of 42 units. Furthermore, we fixed the vertical degrees of freedom for the outer boundary of the plate. The analysis is performed under plane strain conditions and the specimen is discretized with 1800 four-noded standard displacement elements. The three different orientations of the preferred direction are

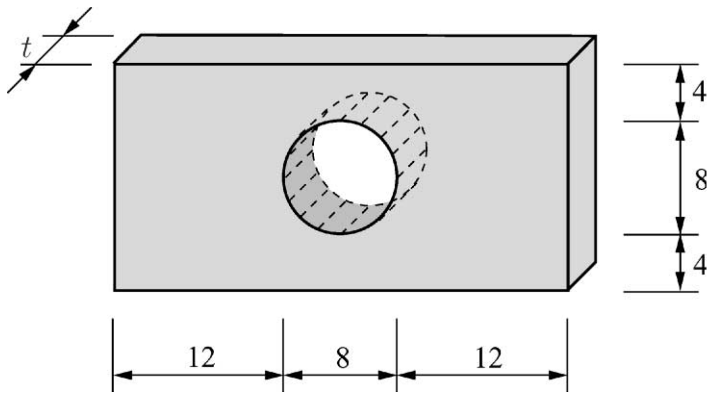


Fig. 7. Geometric properties of the rectangular plate with centered hole.

$$\boldsymbol{a}_1 = (1,1,0)^{\mathrm{T}}/\sqrt{2}, \quad \boldsymbol{a}_2 = (0.5,1,0)^{\mathrm{T}}/\sqrt{1.25} \quad \text{and} \quad \boldsymbol{a}_3 = (1,0,0)^{\mathrm{T}}. \tag{7.98}$$

The chosen free energy function $\psi$ consists again of seven additive terms $\tilde{\psi}_j$ and we set

$$\psi = \sum_{j=1}^{7} \tilde{\psi}_j(I_1, I_2, I_3, J_4, J_5) \quad \text{with } \tilde{\psi}_j | j = 1,\ldots,7 = \psi_i | i = 1, 10, 24, 28, 30, 32, 33. \tag{7.99}$$

In the next equation we summarize the explicit expressions of the chosen ansatz functions:

$$\left.\begin{array}{l} \tilde{\psi}_1(I_1) = \alpha_1 \mathrm{tr}\boldsymbol{C} \\ \tilde{\psi}_2(I_3) = -\delta_2 \ln[\sqrt{\det \boldsymbol{C}}] \\ \tilde{\psi}_3(I_1, I_2, J_4, J_5) = \gamma_5 (\mathrm{tr}[\boldsymbol{M}\mathrm{Cof}\boldsymbol{C}])^3 \\ \tilde{\psi}_4(I_1, J_4) = \phi_2 (\mathrm{tr}[\boldsymbol{D}\boldsymbol{C}])^2 \\ \tilde{\psi}_5(I_1, J_4, J_5) = \phi_4 (\mathrm{tr}[\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}])^2 \\ \tilde{\psi}_6(I_1, I_3, J_4, J_5) = \phi_6 \mathrm{tr}[\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}]/(\det \boldsymbol{C})^{1/3} \\ \tilde{\psi}_7(I_1, I_3, J_4, J_5) = \phi_7 (\mathrm{tr}[\boldsymbol{D}\boldsymbol{C}])^2/(\det \boldsymbol{C})^{1/3} \end{array}\right\}. \tag{7.100}$$

For the simulations we choose for the material parameters in (7.100) the values

$$\left.\begin{array}{l} \alpha_1 = 14.0625, \quad \delta_2 = 325.0, \quad \gamma_5 = 3.64583 \\ \phi_2 = 3.515625, \quad \phi_4 = 20.3125, \quad \phi_6 = 4.6875, \quad \phi_7 = 15.234375 \end{array}\right\}. \tag{7.101}$$

The free energy function (7.99) with the parameters (7.101) is referred to as the material parameter set 2 (**MS 2**). Choosing the $X_3$-axis as the preferred direction we obtain the corresponding linearized moduli at the reference configuration

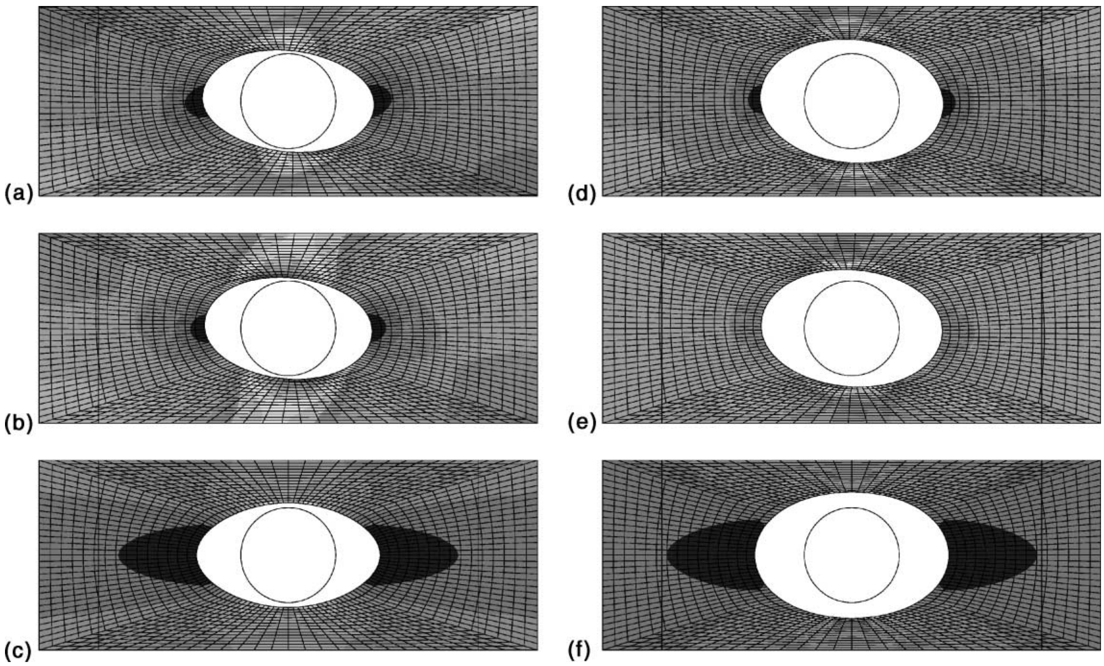


Fig. 8. Tension of a rectangular plate with centered hole. Deformed configurations for material parameter set **MS 1**: (a) $\boldsymbol{a}_1$, (b) $\boldsymbol{a}_2$ and (c) $\boldsymbol{a}_3$, and material parameter set **MS 2**: (d) $\boldsymbol{a}_1$, (e) $\boldsymbol{a}_2$ and (f) $\boldsymbol{a}_3$, respectively.

$$\mathbb{C}_{11} \approx 1000.0, \quad \mathbb{C}_{12} \approx 300.0, \quad \mathbb{C}_{13} \approx 600.0, \quad \mathbb{C}_{33} \approx 1400.0, \quad \mathbb{C}_{44} \approx 200.0. \tag{7.102}$$

Fig. 8a–c depicts the deformed configurations at the final state for the material parameter set **MS 1** and Fig. 8d–f those for the material parameter set **MS 2** for three different orientations $\boldsymbol{a}_i$, $i = 1, 2, 3$ of the rotational symmetry axis. For the non-aligned preferred direction with respect to the symmetry planes of the plate the hole is deformed to a rotated ellipse, see Fig. 8a, b, d, e. For the orientation $\boldsymbol{a}_3$ the principal axes of the ellipse coincide with the symmetry planes of the specimen and the loading conditions. A remarkable difference for the two material sets can be seen by comparing the expansion of the hole. For the first parameter set the area of the final hole is much smaller than it is for the second parameter set.

## 8. Conclusion

In this paper we have proposed the formulation of polyconvex transversely isotropic hyperelasticity in an invariant setting. The constitutive models are based on the Clausius–Planck inequality, so the thermodynamic consistency is guaranteed. The main goal of this work has been the construction of polyconvex anisotropic functions in the sense of Ball in order to guarantee the existence of minimizers of variational principles in finite elasticity. For the free energy we have assumed an additive structure, i.e. it has been built by the sum of additively decoupled terms. Each of these individual isotropic and anisotropic ansatz functions fulfills the polyconvexity condition. The proofs of the polyconvexity for all proposed functions have been given in detail and we have pointed out that several transversely isotropic free energies proposed in the literature do not meet this condition. Furthermore, we have shown that the often used polynomial mixed invariants $J_5$ and $I_1 J_4$ are not polyconvex. The construction of some polyconvex polynomial mixed invariants has been motivated by certain physical interpretations and realized by use of the Cayley-Hamilton theorem. One interesting result is the polyconvexity of the powers of the quadratic mixed invariant with respect to the cofactor of the right Cauchy–Green tensor. This term controls the deformation of a preferred area element of an infinitesimal volume of the body. For the simulation of some model problems the individual free energy terms can be additively merged so that in this class a wide variety of ratios of anisotropy can be modeled. An extension of the proposed formulation to the case of orthotropic material response is given. Here a variety of terms are already given by interchanging the one preferred direction of the transversely isotropic case with the three perpendicular preferred directions of the orthotropic material. Additional terms have been constructed by the powers of linear convex combinations of polyconvex functions.

## Appendix A. Proof of basic properties

In this part of the paper we investigate the polyconvexity conditions alluded to above. We focus our attention on constitutive issues rather than existence theorems in Sobolev spaces. Therefore we do not address growth conditions on the free energy. They can be met by a judicious choice of appearing parameters. Whereas the whole formalism derived up to now could be based on considerations pertaining to the right Cauchy–Green tensor $C = F^{\mathrm{T}}F$ the investigation of conditions like polyconvexity, quasiconvexity and ellipticity are directly based on expressions defined on the deformation gradient $F$. Since we are interested in applications to finite elasticity we restrict ourselves to three space dimensions. Our aim here is to leave the presentation sufficiently selfcontained.

We begin with some simple observations which facilitate the further proofs allowing henceforth to restrict indicial calculations to a minimum.

**Lemma A.1** (Scalar product). *Let* $A$, $B \in \mathbb{M}^{3\times 3}$ *then*

$$\langle A, B\rangle := \operatorname{tr}(AB^{\mathrm{T}})$$

*defines a scalar product on* $\mathbb{M}^{3\times 3}$ *with induced Frobenius matrix norm*

$$\|A\|^2 = \langle A, A\rangle.$$

**Proof.** Standard. □

**Corollary A.2** (Properties of the scalar product). *Let* $A$, $B$, $C \in \mathbb{M}^{3\times 3}$ *and* $\xi \in \mathbb{R}^3$ *then*

1. $\|AB\| \leqslant \|A\|\|B\|$.
2. $\|A.\xi\|_{\mathbb{R}^3} \leqslant \|A\|\|\xi\|_{\mathbb{R}^3}$.
3. $\langle A, BC\rangle = \langle AC^{\mathrm{T}}, B\rangle = \langle B^{\mathrm{T}}A, C\rangle$.

**Proof.** Standard. □

**Lemma A.3.** *Let* $A \in GL(3,\mathbb{R})$. *Then*

$$\forall F \in \mathbb{M}^{3\times 3} \quad \|AF\|^2 \geqslant \lambda_{\min}(A^{\mathrm{T}}A)\|F\|^2.$$

**Proof.** Some easy algebra. □

Let $\eta$, $\xi \in \mathbb{R}^3$, then $\eta \otimes \xi \in \mathbb{M}^{3\times 3}$ and $(\eta \otimes \xi)_{ij} = \eta_i \xi_j$. This yields the following

**Lemma A.4** (Basic properties of the tensor product). *Let* $A \in \mathbb{M}^{3\times 3}$, $v \in \mathbb{R}^3$ *and* $\eta \otimes \xi \in \mathbb{M}^{3\times 3}$ *then*

1. $(\eta \otimes \xi).v = \eta\langle \xi, v\rangle_{\mathbb{R}^3}$.
2. $(\eta \otimes \xi)^{\mathrm{T}} = \xi \otimes \eta$.
3. $\operatorname{trace}(\eta \otimes \xi) = \langle \eta, \xi\rangle_{\mathbb{R}^3}$.
4. $\operatorname{trace}(\eta \otimes \eta) = \|\eta\|^2_{\mathbb{R}^3}$.
5. $\|\eta \otimes \xi\|^2 = \|\eta\|^2_{\mathbb{R}^3}\|\xi\|^2_{\mathbb{R}^3}$.
6. $\langle \eta \otimes \xi, (\eta \otimes \xi)^{\mathrm{T}}\rangle = \langle \eta \otimes \xi, (\xi \otimes \eta)\rangle = \langle \eta, \xi\rangle^2_{\mathbb{R}^3} \geqslant 0$.
7. $\operatorname{trace}((\eta \otimes \xi)^2)) = (\operatorname{trace}(\eta \otimes \xi))^2$.
8. $\|(\eta \otimes \xi)^{\mathrm{T}} + (\eta \otimes \xi)\|^2 \geqslant 2\|\eta\|^2_{\mathbb{R}^3}\|\xi\|^2_{\mathbb{R}^3}$.
9. $A(\eta \otimes \xi) = A.\eta \otimes \xi$.
10. $(\eta \otimes \xi)A = \eta \otimes A^{\mathrm{T}}.\xi$.
11. $A(\eta \otimes \xi)A^{\mathrm{T}} = A.\eta \otimes A.\xi$.
12. $\operatorname{rank}(\eta \otimes \xi) = 1$.
13. *For every matrix* $A \in \mathbb{M}^{3\times 3}$ *with* $\operatorname{rank}(A) = 1$ *there exist vectors* $\eta$, $\xi \in \mathbb{R}^3$ *such that* $A = \eta \otimes \xi$.
14. $B = \mathbb{1} + \eta \otimes \xi \Rightarrow B^{-1} = \mathbb{1} - \frac{1}{1+\langle \eta, \xi\rangle}\eta \otimes \xi$ *if* $\langle \eta, \xi\rangle \neq 1$.

*A.1. Adjugate and determinant*

**Definition A.5** (*Adjugate* $\mathrm{Adj}\,F = \mathrm{Cof}(F)^{\mathrm{T}}$).

$$D(\mathrm{Adj}\,F).H = \mathrm{Adj}\,F\{\langle F^{-T}, H\rangle \mathbb{1} - HF^{-1}\}, \tag{A.1}$$

$$D^2(\mathrm{Adj}\,F).(H,H) = 2\mathrm{Adj}\,H, \tag{A.2}$$

since $\mathrm{Adj}\,F$ is a quadratic expression. The same expansion can be done with the determinant. For $H \in \mathbb{M}^{3\times 3}$ we get after some computations

$$\det(\mathbb{1} + H) = 1 + \mathrm{tr}(H) + \mathrm{tr}(\mathrm{Adj}\,H) + \det H.$$

**Lemma A.6** (Properties of the Adjugate). *Let $A$, $B$, $P \in Gl(3,\mathbb{R})$ and $Q \in O(3)$. Then we have*:

1. $\mathrm{Adj}\,(\xi \otimes \eta) = 0.$
2. $\mathrm{Adj}\,(\mathbb{1} + \xi \otimes \eta) = \mathbb{1} + \langle \xi, \eta\rangle \mathbb{1} - \xi \otimes \eta.$
3. $\mathrm{Adj}\,(AB) = \mathrm{Adj}\,B\ \mathrm{Adj}\,A.$
4. $\mathrm{Adj}\,A^{\mathrm{T}} = (\mathrm{Adj}\,A)^{\mathrm{T}}.$
5. $\mathrm{Adj}\,A\,A^{-1} = \det A\mathbb{1}.$
6. $\mathrm{Adj}\,(P^{-1}AP) = P^{-1}\mathrm{Adj}\,AP$, *hence* Adj *is an isotropic tensor function.*
7. $\mathrm{Adj}\,(A^{-1}) = (\mathrm{Adj}\,A)^{-1}.$
8. *Let $D$ be a diagonal matrix, then* $\mathrm{Adj}\,D = \begin{pmatrix} \lambda_2\lambda_3 & 0 & 0 \\ 0 & \lambda_1\lambda_3 & 0 \\ 0 & 0 & \lambda_1\lambda_2 \end{pmatrix}.$
9. $\mathrm{trace}(\mathrm{Adj}\,D) = \lambda_2\lambda_3 + \lambda_1\lambda_3 + \lambda_1\lambda_2.$
10. $\mathrm{trace}(\mathrm{Adj}\,(P^{-1}AP)) = \mathrm{trace}(\mathrm{Adj}\,A).$
11. $\|\mathrm{Adj}\,(Q^{-1}AQ)\|^2 = \|\mathrm{Adj}\,A\|^2.$
12. $\langle \mathrm{Adj}\,F^{\mathrm{T}}F, \mathbb{1}\rangle = \|\mathrm{Adj}\,F\|^2.$
13. *For $Q \in O(3)$ :* $\mathrm{Adj}\,(QF) = (\mathrm{Adj}\,F)Q^{\mathrm{T}}$ *and* $\|\mathrm{Adj}\,(QF)\| = \|\mathrm{Adj}\,F\|.$

**Remark A.7.** The above properties carry over to non-invertible matrices as well.

**Theorem A.8** (Cayley-Hamilton). *Let $A \in \mathbb{M}^{3\times 3}$. Then $A$ is solution of its characteristic polynomial* $\det(\lambda\mathbb{1} - A) = 0$, *i.e.*

$$0 = \lambda^3 - \mathrm{trace}(A)\lambda^2 + \mathrm{trace}(\mathrm{Adj}\,A)\lambda - \det A\lambda^0$$

*which means*

$$0 = A^3 - \mathrm{trace}(A)A^2 + \mathrm{trace}(\mathrm{Adj}\,A)A - \det A\mathbb{1}. \tag{A.3}$$

**Proof.** Standard exercise. □

**Lemma A.9** (Invariants). *For all real diagonalizable $A \in \mathbb{M}^{3\times 3}$ we set*

$$I_1(A) := \mathrm{tr}(A) = \lambda_1 + \lambda_2 + \lambda_3$$
$$I_2(A) := \mathrm{tr}(\mathrm{Adj}\,A) = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3$$
$$I_3(A) := \det A = \lambda_1\lambda_2\lambda_3.$$

*Because of Theorem* A.8 *this implies*

$$\operatorname{tr}(F)^2 = \operatorname{tr}(F^2) + 2\operatorname{tr}(\operatorname{Adj} F)$$
$$(\lambda_1 + \lambda_2 + \lambda_3)^2 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + 2(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3). \quad \square$$

**Lemma A.10** (Coefficients of the characteristic polynomial)**.** *Let $A$ be real diagonalizable and assume that* $\det A \geqslant 0$. *Then we have*

$$I_1^2(A) \geqslant 3I_2(A)$$
$$I_2^2(A) \geqslant 3I_1(A)I_3(A).$$

**Proof.** Young's inequality shows that $\lambda_i\lambda_j \leqslant (1/2)\lambda_i^2 + (1/2)\lambda_j^2$. Therefore $\lambda_1^2 + \lambda_2^2 + \lambda_3^2 \geqslant \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3$. Hence

$$(\lambda_1 + \lambda_2 + \lambda_3)^2 = (\lambda_1^2 + \lambda_2^2 + \lambda_3^2) + 2(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3) \geqslant 3(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3)$$

which proves $I_1(A)^2 \geqslant 3I_2(A)$. In order to prove the second statement note that we may assume $\lambda_i(A) \neq 0$ without loss of generality since otherwise the statement is true anyway. Let therefore $\det A \neq 0$. Then the inverse $A^{-1} \in \mathbb{M}^{3\times 3}$ exists and with the first statement we know $I_1(A^{-1})^2 \geqslant 3I_2(A^{-1})$. Moreover $\hat{\lambda}(A^{-1})_i = 1/\lambda(A)_i$. Therefore

$$\left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3}\right)^2 \geqslant 3\left(\frac{1}{\lambda_1\lambda_2} + \frac{1}{\lambda_2\lambda_3} + \frac{1}{\lambda_3\lambda_1}\right)$$
$$\left(\frac{\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3}{\lambda_1\lambda_2\lambda_3}\right)^2 \geqslant 3\left(\frac{\lambda_1 + \lambda_2 + \lambda_3}{\lambda_1\lambda_2\lambda_3}\right)$$
$$(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3)^2 \geqslant 3(\lambda_1 + \lambda_2 + \lambda_3)(\lambda_1\lambda_2\lambda_3)$$

which is just $I_2(A)^2 \geqslant 3I_1(A)I_3(A)$. $\square$

**Corollary A.11** (Estimates between $\|F\|$, $\|\operatorname{Adj} F\|$ and $\det F$)**.** *Let* $F \in \mathbb{M}^{3\times 3}$. *Then we have*

$$\|F\|^3 \geqslant 3\sqrt{3}\det F$$
$$\|F\|^2 \geqslant \sqrt{3}\|\operatorname{Adj} F\|$$
$$\|\operatorname{Adj} F\|^3 \geqslant 3\sqrt{3}(\det F)^2$$
$$\|F\|^2 = \langle F^{\mathrm{T}}F, \mathbb{1}\rangle \leqslant \sqrt{3}\|F^{\mathrm{T}}F\|.$$

**Proof.** Set $A = F^{\mathrm{T}}F$. The symmetry of $A$ ensures the applicability of the previous Lemma A.10. Thus

$$I_1(A) = I_1(F^{\mathrm{T}}F) = \operatorname{tr}(F^{\mathrm{T}}F) = \|F\|^2$$
$$I_2(A) = I_2(F^{\mathrm{T}}F) = \operatorname{tr}(\operatorname{Adj}(F^{\mathrm{T}}F)) = \operatorname{tr}(\operatorname{Adj} F \operatorname{Adj} F^{\mathrm{T}}) = \|\operatorname{Adj} F\|^2$$
$$I_3(A) = I_3(F^{\mathrm{T}}F) = \det F^{\mathrm{T}}F = (\det F)^2$$

and also

$$I_1^2(A) \geqslant 3I_2(A) \iff \|F\|^2 \geqslant \sqrt{3}\|\mathrm{Adj}\,F\|$$
$$I_2^2(A) \geqslant 3I_1(A)I_3(A) \iff \|\mathrm{Adj}\,F\|^2 \geqslant \sqrt{3}\|F\|\det F.$$

The last two lines lead immediately to the second statement. The last statement is only a simple algebraic estimate. □

**Lemma A.12** (Properties of the anisotropy structural tensor $M$). *Let $\eta \in \mathbb{R}^3$ with $\|\eta\| = 1$ and define $M = \eta \otimes \eta$. Then the following statements hold*:

1. $M^T = M$.
2. *$M$ is positive semi-definite.*
3. $M^T M = M$.
4. $\mathrm{tr}(M) = 1$.
5. $M^2 = M$.
6. $\|M\|^2 = 1$.
7. $\|\mathbb{1} - M\|^2 = 2$.
8. $(\mathbb{1} - M)(\mathbb{1} - M) = \mathbb{1} - M$.
9. $(\mathbb{1} - M)^T(\mathbb{1} - M) = \mathbb{1} - M$.
10. $(\mathbb{1} - M)$ *is positive semi-definite.*
11. $\mathrm{rank}(M) = 1$.
12. $\mathrm{Adj}\,M = 0$.
13. $\mathrm{rank}(\mathbb{1} - M) = 2$ *and* $\mathrm{Adj}(\mathbb{1} - M) \neq 0$.
14. $\mathrm{Adj}(\mathbb{1} - M) = M$.
15. $\langle H, H.M \rangle \geqslant 0$.

**Lemma A.13** (Formal 2nd derivative of $\Psi(F) := W(F^T F)$). *Let $W : P\mathbb{S}\mathrm{ym}(3) \mapsto \mathbb{R}$. Then the second derivative of $\Psi(F) := W(F^T F)$ verifies*

$$D^2\Psi(F).(H,H) = 2\langle \partial_C W(F^T F), H^T H\rangle + \partial_C^2 W(F^T F).(F^T H + H^T F, F^T H + H^T F)$$

**Proof.** Standard exercise. □

## Appendix B. General convexity conditions

**Definition B.1** (*Convexity*). Let $K$ be a convex set and let $W : K \mapsto \mathbb{R}$. We say that $W$ is convex if

$$W(\lambda F_1 + (1-\lambda)F_2) \leqslant \lambda W(F_1) + (1-\lambda)W(F_2)$$

for all $F_1$, $F_2 \in K$ and $\lambda \in (0,1)$.

**Remark B.2.** Observe that in this definition it is necessary to have the function $W$ be defined on a convex set $K$.

**Lemma B.3** (2nd derivative and convexity). *Let $K$ be a convex set and let $W : K \mapsto \mathbb{R}$ be two times differentiable. Then the following statements are equivalent.*

1. *$W$ is convex.*
2. $D^2 W(F).(H,H) \geqslant 0 \ \forall F \in K, \forall H \in \mathrm{Lin}(K)$,

*where* $\mathrm{Lin}(K)$ *is the linear hull of $K$.*

**Proof.** Rockafellar (1970), page 27. □

**Remark B.4.** In order that $W : K \mapsto \mathbb{R}$ be convex it is not sufficient to assume only

$$D^2W(F).(H,H) \geqslant 0$$

for all $F \in K$, $\forall H \in K$. Since for example with $W : P\mathbb{S}\mathrm{ym} \mapsto \mathbb{R}$, $W(C) = \det C$ we have that $K = P\mathbb{S}\mathrm{ym}$ is a convex set (cone) and

$$D^2W(C).(H,H) = 2\langle C, \mathrm{Adj}\, H\rangle \geqslant 0$$

for $C$, $H \in P\mathbb{S}\mathrm{ym}$, but $W(C) = \det C$ is not convex as a function of $C$.

**Lemma B.5** (Convexity on $\mathbb{M}^{3\times 3}$ and $P\mathbb{S}\mathrm{ym}(3)$)**.** *Let $C \in P\mathbb{S}\mathrm{ym}(3)$ and $W : P\mathbb{S}\mathrm{ym}(3) \mapsto \mathbb{R}$ and assume that $\forall H \in \mathbb{S}\mathrm{ym}(3) : D_C^2\psi(C).(H,H) \geqslant 0$ and $D_C\psi(C) \in P\mathbb{S}\mathrm{ym}_0(3)$. Then the function*

$$W : \mathbb{M}^{3\times 3} \mapsto \mathbb{R}, \quad F \mapsto W(F) := \psi(F^{\mathrm{T}}F) \tag{B.1}$$

*is convex.*

**Proof.** Use Lemma A.13 for the second derivative of $W$ and observe that

$$\mathrm{Lin}(P\mathbb{S}\mathrm{ym}) = \mathbb{S}\mathrm{ym}.$$

Apply then basic properties of the scalar product. □

**Lemma B.6** (Convexity of the square). *Let $P : \mathbb{R}^n \mapsto \mathbb{R}$ be convex and $P(Z) \geqslant 0$. Then the function*

$$Z \in \mathbb{R}^n \mapsto [P(Z)][P(Z)]$$

*is convex.*

**Proof.** Assume first that $P$ is a smooth function. The second differential of $E(Z) = P(Z)P(Z)$ can be easily calculated. We get

$$D_ZE(Z).H = P(Z)D_ZP(Z).H + D_ZP(Z).HP(Z)$$
$$D_Z^2E(Z).(H,H) = 2\big(P(Z)D_Z^2P(Z).(H,H) + D_ZP(Z).HD_ZP(Z).H\big) \geqslant 0.$$

Hence $E(Z)$ is convex. In the non-smooth case we proceed as follows:

$$E(\lambda Z_1 + (1-\lambda)Z_2) = [P(\lambda Z_1 + (1-\lambda)Z_2)][P(\lambda Z_1 + (1-\lambda)Z_2)].$$

The assumed convexity of $P$ shows that

$$[P(\lambda Z_1 + (1-\lambda)Z_2)] \leqslant [\lambda P(Z_1) + (1-\lambda)P(Z_2)].$$

Since the square function is a monotone increasing function for positive values and assuming that $[\lambda P(Z_1) + (1-\lambda)P(Z_2)]$ is positive we get the estimate

$$E(\lambda Z_1 + (1-\lambda)Z_2) \leqslant [\lambda P(Z_1) + (1-\lambda)P(Z_2)]^2.$$

However, since the square function is itself convex we may proceed to write

$$E(\lambda Z_1 + (1-\lambda)Z_2) \leqslant \lambda P(Z_1)^2 + (1-\lambda)P(Z_2)^2 = \lambda E(Z_1) + (1-\lambda)E(Z_2).$$

The proof is complete. □

**Corollary B.7.** *Let $P : \mathbb{R}^n \mapsto \mathbb{R}$ be convex and assume that $P(Z) \geqslant 0$. Then the function*

$$Z \in \mathbb{R}^n \mapsto [P(Z)]^p, \quad p \geqslant 1$$

*is convex.*

**Proof.** The same ideas as before carry over to this situation. □

**Remark B.8** (*Nonconvexity of mixed products*). Let $P_i : \mathbb{R}^n \mapsto \mathbb{R}$, $i = 1, 2$ be convex and assume $P_i \geqslant 0$. Then the function

$$Z \in \mathbb{R}^n \mapsto [P_1(Z)][P_2(Z)]$$

is in general non-convex.

**Lemma B.9** (Convexity and monotone composition). *Let $P : \mathbb{R}^n \mapsto \mathbb{R}$ be convex and let $m : \mathbb{R} \mapsto \mathbb{R}$ be convex and monotone increasing. Then the function $\mathbb{R}^n \mapsto \mathbb{R}$, $X \mapsto m(P(X))$ is convex.*

**Proof.** A direct check of the convexity condition. □

## Appendix C. Convexity of special terms

**Lemma C.1** (Isochoric terms). *Let $W(F) = \|F\|^2 / \det F^{\frac{2}{3}}$. Then $W$ is polyconvex.*

**Proof.** We investigate first the convexity of the function $P : \mathbb{R}^+ \times \mathbb{R} \mapsto \mathbb{R}$, $P(x, y) = f(x)g(y)$. The matrix of second derivatives is of course

$$D^2P(x,y) = \begin{pmatrix} f''(x)g(y) & f'(x)g'(y) \\ f'(x)g'(y) & f(x)g''(y) \end{pmatrix}.$$

If $f$, $g$ are positive, smooth and convex then we have $f''(x)g(y) \geqslant 0$ and $\det D^2P(x,y) = f''(x)g(y)f(x) \times g''(y) - (f'(x)g'(x))^2$. Observe that $P$ is convex, if $D^2P$ is positive definite by Lemma B.3. In our situation $D^2P$ is positive definite, if $f''(x)g(y) \geqslant 0$ and $\det D^2P(x,y) \geqslant 0$. Thus we must guarantee that $f''(x)g(y)f(x)g''(y) \geqslant (f'(x)g'(x))^2$.

Let $\alpha > 0$ and $p \geqslant 2$. We choose $f(x) = x^{-\alpha}$ and $g(y) = y^p$. Then

$$f''(x)g(y)f(x)g''(y) = \alpha(\alpha+1)x^{-(2+\alpha)}y^p x^{-\alpha} p(p-1)y^{p-2}$$

and

$$(f'(x)g'(x))^2 = (-\alpha x^{-(\alpha+1)} p y^{p-1})^2 = \alpha^2 x^{-2(\alpha+1)} p^2 y^{2(p-1)}.$$

We arrive at the condition that

$$\frac{\alpha+1}{\alpha} \geqslant \frac{p}{p-1}. \tag{C.1}$$

The larger one chooses $p$, the better for the choice of $\alpha$. Notably $P(x,y) = (1/x^\alpha)y^p$ is convex for $\alpha = 2/3$ and $p = 2$. We set

$$\widehat{W}(F, \xi) = P(\xi, \|F\|) = \frac{\|F\|^2}{\xi^{\frac{2}{3}}}.$$

We check the convexity of $\widehat{W}(F,\xi)$. Thus

$$\widehat{W}(\lambda F_1+(1-\lambda)F_2,\lambda\xi_1+(1-\lambda)\xi_2)=P(\lambda\xi_1+(1-\lambda)\xi_2,\|\lambda F_1+(1-\lambda)F_2\|)=\frac{\|\lambda F_1+(1-\lambda)F_2\|^2}{(\lambda\xi_1+(1-\lambda)\xi_2)^{\frac{2}{3}}}$$

and the monotonicity of the square function for positive arguments yields

$$\widehat{W}(\lambda F_1+(1-\lambda)F_2,\lambda\xi_1+(1-\lambda)\xi_2)\leqslant\frac{(\lambda\|F_1\|+(1-\lambda)\|F_2\|)^2}{(\lambda\xi_1+(1-\lambda)\xi_2)^{\frac{2}{3}}}=P(\lambda\xi_1+(1-\lambda)\xi_2,\lambda\|F_1\|+(1-\lambda)\|F_2\|).$$

Since by assumption $P$ is convex, we get

$$\begin{aligned}&\widehat{W}(\lambda F_1+(1-\lambda)F_2,\lambda\xi_1+(1-\lambda)\xi_2)\leqslant\lambda P(\xi_1,\|F_1\|)+(1-\lambda)P(\xi_2,\|F_2\|)\\&\quad=\lambda\widehat{W}(F_1,\xi_1)+(1-\lambda)\widehat{W}(F_2,\xi_2).\end{aligned}$$

Now recall the extension of $W$ to all of $\mathbb{M}^{3\times3}$ and use (3.29). Thus we have shown that $\widehat{W}$ is convex on the convex set $\mathbb{M}^{3\times3}\times\mathbb{R}^+$ and convexly extended to $\mathbb{M}^{3\times3}\times\mathbb{R}$. The proof is complete (see also Dacorogna, 1989, page 140). □

**Lemma C.2** (Convex terms). *Let $X\in\mathbb{M}^{3\times3}$ and $M=\eta\otimes\eta$. Then the following terms are each convex as functions in $X$:*

1. $X\mapsto[\mathrm{tr}(X^TXM)]^k, k\geqslant1.$
2. $X\mapsto[\mathrm{tr}(X^TX(\mathbb{1}-M))]^k, k\geqslant1.$
3. $X\mapsto[\mathrm{tr}(X^TXMX^TXM)]^k, k\geqslant1.$
4. $X\mapsto[\mathrm{tr}(X^TX)]^2+\mathrm{tr}(X^TX)\mathrm{tr}(X^TXM).$
5. $X\mapsto2[\mathrm{tr}(X^TX)]^2+\mathrm{tr}(X^TX)\mathrm{tr}(X^TX(\mathbb{1}-M)).$
6. $X\mapsto\frac{1}{2}[\mathrm{tr}(X^TX)]^2+\mathrm{tr}(X^TXX^TXM),$

*and the statements remain true if $X$ is changed into $X^T$ since linear transformations leave convexity properties invariant.*

**Proof.** 1. $[\mathrm{tr}(X^TXM)]^k=\langle X,XM\rangle^k$. We compute the second differential:

$$\begin{aligned}&D_X\Big(\langle X,XM\rangle^k\Big).H=k\langle X,XM\rangle^{k-1}(\langle X,HM\rangle+\langle H,XM\rangle)=2k\langle X,XM\rangle^{k-1}\langle X,HM\rangle\\&D_X^2\Big(\langle X,XM\rangle^k\Big).(H,H)=4k(k-1)\langle X,XM\rangle^{k-2}\langle XM,H\rangle^2+2k\langle X,XM\rangle^{k-1}\langle H,HM\rangle\geqslant0\end{aligned}$$

in this context see also A.12 Eq. (15).

2. $[\mathrm{tr}(X^TX(\mathbb{1}-M))]^k=\Big(\|X\|^2-\|X.\eta\|^2_{\mathbb{R}^3}\Big)^k$. We may apply the same reasoning as in the previous line. Observe that

$$\Big(\|X\|^2-\|X.\eta\|^2\Big)\geqslant0\quad\text{if }\|\eta\|=1.$$

3.

$$\begin{aligned}(\mathrm{tr}[X^TXMX^TXM])^k&=\langle X^TXM,MX^TX\rangle^k=\langle X^TX(\eta\otimes\eta),(\eta\otimes\eta)X^TX\rangle^k\\&=\langle X^T(X.\eta\otimes\eta),(\eta\otimes X.\eta)X\rangle^k=\langle(X.\eta\otimes\eta)X^T,X(\eta\otimes X.\eta)\rangle^k\\&=\langle(X.\eta\otimes X.\eta),(X.\eta\otimes X.\eta)\rangle^k=\|(X.\eta\otimes X.\eta)\|^{2k}=\|X.\eta\|^{4k}_{\mathbb{R}^3}.\end{aligned}$$

Hence, computing the differentials yields

$$D_X\left(\|X.\eta\|^{4k}_{\mathbb{R}^3}\right).H = 4k\|X.\eta\|^{4k-2}_{\mathbb{R}^3}\langle X.\eta, H.\eta\rangle_{\mathbb{R}^3}$$

$$D^2_X\left(\|X.\eta\|^{4k}_{\mathbb{R}^3}\right).(H,H) = 4k(4k-2)\|X.\eta\|^{4k-4}_{\mathbb{R}^3}\langle X.\eta, H.\eta\rangle^2_{\mathbb{R}^3} + 4k\|X.\eta\|^{4k-2}_{\mathbb{R}^3}\langle H.\eta, H.\eta\rangle_{\mathbb{R}^3} \geqslant 0.$$

4. $\mathrm{tr}(X^\mathrm{T}X)^2 + \mathrm{tr}(X^\mathrm{T}X)\mathrm{tr}(X^\mathrm{T}XM) = \|X\|^4 + \|X\|^2\|X.\eta\|^2_{\mathbb{R}^3}$. We calculate the second differential, which yields

$$\begin{aligned} D^2_X\left(\|X\|^4 + \|X\|^2\|X.\eta\|^2_{\mathbb{R}^3}\right).(H,H) &= 8\langle X,H\rangle^2 + 4\|X\|^2\|H\|^2 + 8\langle X,H\rangle\langle X.\eta, H.\eta\rangle_{\mathbb{R}^3} \\ &\quad + 2\|X.\eta\|^2_{\mathbb{R}^3}\|H\|^2 + 2\|X\|^2\|H.\eta\|^2_{\mathbb{R}^3} \\ &\geqslant 8\langle X,H\rangle^2 + 4\|X\|^2\|H\|^2 - 8(\|X\|\|H.\eta\|_{\mathbb{R}^3})(\|H\|\|X.\eta\|_{\mathbb{R}^3}) \\ &\quad + 2\|X.\eta\|^2_{\mathbb{R}^3}\|H\|^2 + 2\|X\|^2\|H.\eta\|^2_{\mathbb{R}^3} \\ &\geqslant 8\langle X,H\rangle^2 + 4\|X\|^2\|H\|^2 \\ &\quad - 4\|X\|^2\|H.\eta\|^2_{\mathbb{R}^3} - 4\|H\|^2\|X.\eta\|^2_{\mathbb{R}^3} + 2\|X.\eta\|^2_{\mathbb{R}^3}\|H\|^2 + 2\|X\|^2\|H.\eta\|^2_{\mathbb{R}^3} \\ &\geqslant 8\langle X,H\rangle^2 + 4\|X\|^2\|H\|^2 - 2\|X\|^2\|H.\eta\|^2_{\mathbb{R}^3} - 2\|H\|^2\|X.\eta\|^2_{\mathbb{R}^3} \\ &\geqslant 8\langle X,H\rangle^2 \geqslant 0, \end{aligned}$$

where we have used Young's inequality.

5. $X \mapsto 2[\mathrm{tr}(X^\mathrm{T}X)]^2 + \mathrm{tr}(X^\mathrm{T}X)\mathrm{tr}(X^\mathrm{T}X(\mathbb{1} - M)) = 2\|X\|^4 + \|X\|^2\|X(\mathbb{1} - M)\|^2$. We calculate the second differential, which yields

$$\begin{aligned} D^2_X\left(2\|X\|^4 + \|X\|^2\|X(\mathbb{1}-M)\|^2\right).(H,H) &= 16\langle X,H\rangle^2 + 8\|X\|^2\|H\|^2 + 8\langle X,H\rangle\langle X(\mathbb{1}-M), H(\mathbb{1}-M)\rangle \\ &\quad + 2\|X(\mathbb{1}-M)\|^2\|H\|^2 + 2\|X\|^2\|H(\mathbb{1}-M)\|^2 \\ &\geqslant 16\langle X,H\rangle^2 + 8\|X\|^2\|H\|^2 - 8\|X\|\|H\|\|X(\mathbb{1}-M)\|\|H(\mathbb{1}-M)\| \\ &\quad + 2\|X(\mathbb{1}-M)\|^2\|H\|^2 + 2\|X\|^2\|H(\mathbb{1}-M)\|^2 \\ &\geqslant 16\langle X,H\rangle^2 + 8\|X\|^2\|H\|^2 - 4\|X\|^2\|H(\mathbb{1}-M)\|^2 \\ &\quad - 4\|H\|^2\|X(\mathbb{1}-M)\|^2 + 2\|X(\mathbb{1}-M)\|^2\|H\|^2 \\ &\quad + 2\|X\|^2\|H(\mathbb{1}-M)\|^2 \\ &\geqslant 16\langle X,H\rangle^2 + 8\|X\|^2\|H\|^2 - 4\|X\|^2\|H\|^2\|(\mathbb{1}-M)\|^2 \\ &\quad - 4\|H\|^2\|X\|^2\|(\mathbb{1}-M)\|^2 + 2\|X(\mathbb{1}-M)\|^2\|H\|^2 + 2\|X\|^2\|H(\mathbb{1}-M\|^2 \\ &\geqslant 16\langle X,H\rangle^2 + 8\|X\|^2\|H\|^2 - 2\|X\|^2\|H\|^2\|(\mathbb{1}-M)\|^2 \\ &\quad - 2\|H\|^2\|X\|^2\|(\mathbb{1}-M)\|^2 \\ &\geqslant 16\langle X,H\rangle^2 + 8\|X\|^2\|H\|^2 - 8\|X\|^2\|H\|^2 = 16\langle X,H\rangle^2 \geqslant 0. \end{aligned}$$

6. $(1/2)[\mathrm{tr}(X^\mathrm{T}X)]^2 + \mathrm{tr}(X^\mathrm{T}XX^\mathrm{T}XM) = (1/2)\|X\|^4 + \|X^\mathrm{T}X.\eta\|^2_{\mathbb{R}^3}$. Compute the differentials

$$D_X\left(\frac{1}{2}\|X\|^4 + \|X^\mathrm{T}X.\eta\|^2_{\mathbb{R}^3}\right).H = 2\|X\|^2\|H\|^2 + \langle X^\mathrm{T}X.\eta, (X^\mathrm{T}H + H^\mathrm{T}X).\eta\rangle_{\mathbb{R}^3}$$

$$\begin{aligned} D^2_X\left(\frac{1}{2}\|X\|^4 + \|X^\mathrm{T}X.\eta\|^2_{\mathbb{R}^3}\right).(H,H) &= 2\|X\|^2\|H\|^2 + 4\langle X,H\rangle^2 + 2\langle X^\mathrm{T}X.\eta, H^\mathrm{T}H.\eta\rangle_{\mathbb{R}^3} \\ &\quad + \|(X^\mathrm{T}H + H^\mathrm{T}X).\eta\|^2_{\mathbb{R}^3} \\ &\geqslant 2\|X\|^2\|H\|^2 + 4\langle X,H\rangle^2 - 2\|X\|^2\|H\|^2\|\eta\|^2_{\mathbb{R}^3} \\ &\quad + \|(X^\mathrm{T}H + H^\mathrm{T}X).\eta\|^2_{\mathbb{R}^3} \\ &= 4\langle X,H\rangle^2 + \|(X^\mathrm{T}H + H^\mathrm{T}X).\eta\|^2_{\mathbb{R}^3} \geqslant 0. \qquad \square \end{aligned}$$

**Lemma C.3** (Generic polyconvex terms). *Let $F \in \mathbb{M}^{3\times 3}$ and $M = \eta \otimes \eta$. Then the following terms are each polyconvex for $k \geqslant 1$:*

$$1.\ \frac{[\mathrm{tr}(F^{\mathrm{T}}F)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}},\quad 2.\ \frac{[\mathrm{tr}(F^{\mathrm{T}}FM)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}},\quad 3.\ \frac{[\mathrm{tr}(F^{\mathrm{T}}F(\mathbb{1}-M))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}}$$

$$4.\ \frac{[\mathrm{tr}(\mathrm{Adj}(F^{\mathrm{T}}F))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}},\quad 5.\ \frac{[\mathrm{tr}(\mathrm{Adj}(F^{\mathrm{T}}F)M)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}},\quad 6.\ \frac{[\mathrm{tr}(\mathrm{Adj}(F^{\mathrm{T}}F)(\mathbb{1}-M))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}}$$

**Proof.**

$$1.\ \frac{[\mathrm{tr}(F^{\mathrm{T}}F)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}} = \frac{\|F\|^{2k}}{(\det F)^{\frac{2}{3}}}$$

and we may use the same ideas as in the proof to Lemma C.1 to conclude that the term is polyconvex.

$$2.\ \frac{[\mathrm{tr}(F^{\mathrm{T}}FM)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}} = \frac{\langle F, FM\rangle^k}{(\det F)^{\frac{2}{3}}} = \frac{\langle F, F(\eta\otimes\eta)\rangle^k}{(\det F)^{\frac{2}{3}}} = \frac{\|F.\eta\|^{2k}}{(\det F)^{\frac{2}{3}}}.$$

We have already shown (see Eq. (C.1)) that the function $P(x,y) = (1/x^{\alpha})y^p$ is convex provided that $\alpha = 2/3$ and $p = 2k \geqslant 2$. Now define a new function

$$\widehat{W}(F,\zeta) := P(\zeta, \|F.\eta\|) = \frac{\|F.\eta\|^{2k}}{\zeta^{\frac{2}{3}}}.$$

Observe that by the monotonicity of the square for positive arguments we have the inequality

$$\|\lambda F_1.\eta + (1-\lambda)F_2.\eta\|^{2k} \leqslant (\lambda\|F_1.\eta\| + (1-\lambda)\|F_2.\eta\|)^{2k}. \tag{C.2}$$

It remains to check the convexity of $\widehat{W}(F,\zeta)$. To this end

$$\begin{aligned}\widehat{W}(\lambda F_1 + (1-\lambda)F_2, \lambda\zeta_1 + (1-\lambda)\zeta_2) &= P(\lambda\zeta_1 + (1-\lambda)\zeta_2, \|\lambda F_1.\eta + (1-\lambda)F_2.\eta\|)\\ &= \frac{\|\lambda F_1.\eta + (1-\lambda)F_2.\eta\|^{2k}}{(\lambda\zeta_1 + (1-\lambda)\zeta_2)^{\frac{2}{3}}}.\end{aligned}$$

With Eq. (C.2) we have

$$\begin{aligned}&\widehat{W}(\lambda F_1 + (1-\lambda)F_2, \lambda\zeta_1 + (1-\lambda)\zeta_2) \leqslant \frac{(\lambda\|F_1.\eta\| + (1-\lambda)\|F_2.\eta\|)^{2k}}{(\lambda\zeta_1 + (1-\lambda)\zeta_2)^{\frac{2}{3}}}\\ &\quad = P(\lambda\zeta_1 + (1-\lambda)\zeta_2, \lambda\|F_1.\eta\| + (1-\lambda)\|F_2.\eta\|).\end{aligned}$$

The convexity of $P$ yields

$$\begin{aligned}&\widehat{W}(\lambda F_1 + (1-\lambda)F_2, \lambda\zeta_1 + (1-\lambda)\zeta_2) \leqslant \lambda P(\zeta, \|F_1.\eta\|) + (1-\lambda)P(\zeta_2, \|F_2.\eta\|)\\ &\quad = \lambda\widehat{W}(F_1,\zeta_1) + (1-\lambda)\widehat{W}(F_2,\zeta_2).\end{aligned}$$

The proof is finished bearing the correct extension (3.29) in mind.

$$3.\ \frac{[\mathrm{tr}(F^{\mathrm{T}}F(\mathbb{1}-M))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}} = \frac{\|F(\mathbb{1}-M)\|^{2k}}{(\det F)^{\frac{2}{3}}}$$ and we proceed as in the second case.

4. $\dfrac{[\operatorname{tr}(\operatorname{Adj}(F^{\mathrm{T}}F))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}} = \dfrac{\|\operatorname{Adj}F\|^{2k}}{(\det F)^{\frac{2}{3}}}$ and we proceed as in the first case.

5. $\dfrac{[\operatorname{tr}(\operatorname{Adj}(F^{\mathrm{T}}F)M)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}} = \dfrac{\|\operatorname{Adj}F^{\mathrm{T}}.\eta\|^{2k}}{(\det F)^{\frac{2}{3}}}$ and we proceed as in the second case.

6. $\dfrac{[\operatorname{tr}(\operatorname{Adj}(F^{\mathrm{T}}F)(\mathbb{1}-M))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}} = \dfrac{\|\operatorname{Adj}F^{\mathrm{T}}(\mathbb{1}-M)\|^{2k}}{(\det F)^{\frac{2}{3}}}$ and we proceed as in the second case. □

**Corollary C.4** (Generic exponential polyconvex terms). *Let $F \in \mathbb{M}^{3\times 3}$ and $M = \eta\otimes\eta$. Then the following terms are each polyconvex for $k \geqslant 1$:*

$$1.\ \exp\left[\frac{[\operatorname{tr}(F^{\mathrm{T}}F)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}}\right],\quad 2.\ \exp\left[\frac{[\operatorname{tr}(F^{\mathrm{T}}FM)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}}\right],$$

$$3.\ \exp\left[\frac{[\operatorname{tr}(F^{\mathrm{T}}F(\mathbb{1}-M))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}}\right],\quad 4.\ \exp\left[\frac{[\operatorname{tr}(\operatorname{Adj}(F^{\mathrm{T}}F))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}}\right],$$

$$5.\ \exp\left[\frac{[\operatorname{tr}(\operatorname{Adj}(F^{\mathrm{T}}F)M)]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}}\right],\quad 6.\ \exp\left[\frac{[\operatorname{tr}(\operatorname{Adj}(F^{\mathrm{T}}F)(\mathbb{1}-M))]^k}{(\det[F^{\mathrm{T}}F])^{\frac{1}{3}}}\right],$$

7. $\exp[W(F)]$ *if $W(F)$ is polyconvex.*

**Proof.** By the foregoing lemma each argument of the exponential is polyconvex. Since exp is convex and monotone increasing it preserves the underlying convexity. Hence the composition is polyconvex. Observe, however, that these functions alone are not stress-free in the reference configuration. □

**Lemma C.5** (Special polyconvex terms). *Let $F \in \mathbb{M}^{3\times 3}$. Then the following terms are each polyconvex as functions $F \mapsto \mathbb{R}^+$:*

1. $F \mapsto \left(\dfrac{\|F\|^2}{(\det F)^{\frac{2}{3}}} - 3\right)^i, \quad i \geqslant 1.$

2. $F \mapsto \left(\dfrac{\|\operatorname{Adj}F\|^3}{(\det F)^2} - 3\sqrt{3}\right)^j = \left(\dfrac{\|\operatorname{Adj}F^{\mathrm{T}}\|^3}{(\det F)^2} - 3\sqrt{3}\right)^j, \quad j \geqslant 1.$

**Proof.**

1. We have already checked in Lemma C.1 that the expression $(\|F\|^2/(\det F)^{\frac{2}{3}})$ is polyconvex, hence there exists a convex function $P(F, \det F) = (\|F\|^2/(\det F)^{\frac{2}{3}})$. Observe that by the estimates for the invariants Lemma A.11 we know that $P(F, \det F) - 3 \geqslant 0$. We define the function $[a]_+ = \max\{a, 0\}$. Observe that $x \mapsto \max\{f(x), 0\}$ is convex if $f$ is convex. Then

$$\left(\frac{\|F\|^2}{(\det F)^{\frac{2}{3}}} - 3\right)^i = [P\underbrace{(F, \det F)}_{X\in\mathbb{R}^{10}} - 3]_+^i.$$

$P$ is convex in $X$ and $x \mapsto x^i$, $i \geqslant 1$ is monotone increasing for positive values and convex, hence

$$[P(X) - 3]_+^i$$

is altogether convex in $X$, which is however the polyconvexity of

$$F \mapsto [P(F, \det F) - 3]_+^i.$$

Since this last expression coincides with

$$\left( \frac{\|F\|^2}{(\det F)^{\frac{2}{3}}} - 3 \right)^i$$

the polyconvexity is proved. □

2. We know already that $(\|\operatorname{Adj} F\|^3/(\det F)^2) - 3\sqrt{3}$ is polyconvex since the exponents verify the decisive inequality $(\alpha+1)/\alpha \geqslant p/(p-1)$. Moreover, $\|\operatorname{Adj} F\|^3/(\det F)^2) - 3\sqrt{3} \geqslant 0$ with Lemma A.11. Now exactly the same reasoning as before applies.

**Corollary C.6.** *Let $F \in \mathbb{M}^{3\times 3}$. Then the following more general terms are each polyconvex*:

1. $F \mapsto \left( \frac{\|F\|^{2k}}{(\det F)^{\frac{2k}{3}}} - 3^k \right)^i, \quad i \geqslant 1, \; k \geqslant 1.$

2. $F \mapsto \left( \frac{\|\operatorname{Adj} F\|^{3k}}{(\det F)^{2k}} - (3\sqrt{3})^k \right)^j, \quad j \geqslant 1, \; k \geqslant 1.$

3. $F \mapsto \exp\left[ \left( \frac{\|F\|^{2k}}{(\det F)^{\frac{2k}{3}}} - 3^k \right)^i \right] - 1, \quad i \geqslant 1, \; k \geqslant 1.$

4. $F \mapsto \exp\left[ \left( \frac{\|\operatorname{Adj} F\|^{3k}}{(\det F)^{2k}} - (3\sqrt{3})^k \right)^j \right] - 1, \quad j \geqslant 1, \; k \geqslant 1.$

**Proof.** Apply the same ideas as above and observe that exp is a convex monotone increasing function, so that we may apply Lemma B.9. □

One might be tempted to use some other ansatz terms in order to construct polyconvex strain energies. However, we have e.g.

**Lemma C.7** (Non-elliptic terms I). *Let $F \in \mathbb{M}^{3\times 3}$ and $M = a \otimes a$. Then the following terms are each non-elliptic, hence non-quasiconvex*:

1. $F \mapsto \operatorname{tr}(F^T F M)\operatorname{tr}(F^T F) = \operatorname{tr}(CM)\operatorname{tr}(C).$

2. $F \mapsto \operatorname{tr}(F^T F F^T F M) = \operatorname{tr}(C^2 M).$

3. $F \mapsto \left( \frac{\|\operatorname{Adj} F\|^2}{(\det F)^{\frac{4}{3}}} - 3 \right)^i = \left( \operatorname{tr}\left( \operatorname{Adj}\left( \frac{C}{(\det C)^{\frac{1}{3}}} \right) \right) - 3 \right)^i = \left( \operatorname{tr}\left( \operatorname{Adj}\left( \frac{C}{(\det C)^{\frac{1}{3}}} \right) - \mathbb{1} \right) \right)^i \quad i \geqslant 1.$

**Proof.**

1. See Proof (3).
2. See Proof (5).
3. Even though $\|\mathrm{Adj}\, F\|^2/(\det F)^{\frac{4}{3}} - 3 \geqslant 0$ in light of Lemma A.11, the term $\|\mathrm{Adj}\, F\|^2/(\det F)^{\frac{4}{3}}$ alone does not have the right exponents to be polyconvex. Moreover it can be shown that the term is non-elliptic (Dacorogna, 1989). □

**Lemma C.8** (Non-elliptic terms II). *Let* $F \in \mathbb{M}^{3\times 3}$ *and* $M = a \otimes a$ *with* $\|a\| = 1$. *Then the following terms are each non-elliptic, hence non-quasiconvex*:

1. $F \mapsto \exp\left(\left\langle \frac{C}{(\det C)^{\frac{1}{3}}}, a\otimes a\right\rangle - 1\right) - \left\langle \frac{C}{(\det C)^{\frac{1}{3}}}, a\otimes a\right\rangle.$
2. $F \mapsto \left(\left\langle \frac{C}{(\det C)^{\frac{1}{3}}}, a\otimes a\right\rangle - 1\right)^q, \quad q \geqslant 2.$

*Observe that both terms have stress-free reference configuration.*

**Proof.** We show the non-ellipticity of the first expression. The non-ellipticity of the second one follows along the same lines. We calculate

$$\left\langle \frac{C}{(\det C)^{\frac{1}{3}}}, a\otimes a\right\rangle = \left\langle \frac{F^{\mathrm{T}}F}{(\det F)^{\frac{2}{3}}}, a\otimes a\right\rangle = \frac{1}{(\det F)^{\frac{2}{3}}}\|F.a\|^2.$$

Set $F = F_0 + t\xi\otimes\eta$. This yields

$$\begin{aligned}
\frac{1}{(\det F)^{\frac{2}{3}}}\|F.a\|^2 &= \frac{\|F_0 + t\xi\otimes\eta\|^2}{(\det[F_0 + t\xi\otimes\eta])^{\frac{2}{3}}} = \frac{\|F_0.a + t\xi\langle\eta, a\rangle\|^2}{(\det F_0 + \langle \mathrm{Adj}\, F_0^{\mathrm{T}}, t\xi\otimes\eta\rangle + 0 + 0)^{\frac{2}{3}}} \\
&= \frac{\|F_0.a\|^2 + 2t\langle F_0.a, \xi\rangle\langle\eta, a\rangle + t^2\langle\xi,\xi\rangle\langle\eta, a\rangle}{(\det F_0 + t\langle \mathbb{1}, \mathrm{Adj}\, F_0.\xi\otimes\eta\rangle)^{\frac{2}{3}}} \\
&= \frac{\|F_0.a\|^2 + 2t\langle F_0.a, \xi\rangle\langle\eta, a\rangle + t^2\langle\xi,\xi\rangle\langle\eta, a\rangle}{(\det F_0 + t\langle \mathrm{Adj}\, F_0.\xi, \eta\rangle)^{\frac{2}{3}}}.
\end{aligned}$$

Now we choose

$$a = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix}, \quad \xi = \begin{pmatrix}0\\1\\0\end{pmatrix}, \eta = \begin{pmatrix}1\\0\\0\end{pmatrix}, \quad F_0^{-1} = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\\ \frac{1}{\sqrt{2}} & \frac{3\sqrt{2}}{2} & 0\\ 0 & 0 & d\end{pmatrix}.$$

This yields

$$\begin{aligned}
&\|a\| = \|\xi\| = \|\eta\| = 1,\\
&\langle a, \eta\rangle = \langle a, \xi\rangle = \frac{1}{\sqrt{2}},\\
&\langle \eta, \xi\rangle = 0,\\
&F_0^{-1}.\eta = a, \quad \det F_0 = \frac{1}{d}, \quad F_0.a = \eta\\
&\det F_0 a = \det F_0 F_0^{-1}.\eta = \mathrm{Adj}\, F_0.\eta.
\end{aligned}$$

As a consequence, we get

$$\frac{\|F_0.a\|^2 + 2t\langle F_0.a,\xi\rangle\langle\eta,a\rangle + t^2\langle\xi,\xi\rangle\langle\eta,a\rangle}{(\det F_0 + t\langle \operatorname{Adj} F_0.\xi,\eta\rangle)^{\frac{2}{3}}} = \frac{\|\eta\|^2 + t\langle\eta,\xi\rangle\langle\eta,a\rangle + t^2\langle\xi,\xi\rangle\langle\eta,a\rangle}{\left(\frac{1}{d} + t\langle\xi, \operatorname{Adj} F_0^{\mathrm{T}}.\eta\rangle\right)^{\frac{2}{3}}} = \frac{1+0+t^2\frac{1}{\sqrt{2}}}{\left(\frac{1}{d} + t\langle\xi, \operatorname{Adj} F_0.\eta\rangle\right)^{\frac{2}{3}}}$$
$$= \frac{1+t^2\frac{1}{\sqrt{2}}}{\left(\frac{1}{d} + t\det F_0\langle\xi,a\rangle\right)^{\frac{2}{3}}} = \frac{1+t^2\frac{1}{\sqrt{2}}}{\frac{1}{d^{\frac{2}{3}}}\left(1+t\frac{1}{\sqrt{2}}\right)^{\frac{2}{3}}}.$$

Thus

$$h(t) = W(F_0 + t\xi\otimes\eta) = \exp\left(\frac{1+t^2\frac{1}{\sqrt{2}}}{\frac{1}{d^{\frac{2}{3}}}\left(1+t\frac{1}{\sqrt{2}}\right)^{\frac{2}{3}}} - 1\right) - \frac{1+t^2\frac{1}{\sqrt{2}}}{\frac{1}{d^{\frac{2}{3}}}\left(1+t\frac{1}{\sqrt{2}}\right)^{\frac{2}{3}}}.$$

If we choose $1/d^{\frac{2}{3}} = 3$ it turns out that $h$ is not convex in $t$, hence (Theorem 3.5) $W$ is not elliptic. We remark that the non-ellipticity is mainly due to the fact that

$$\left\langle \frac{C}{(\det C)^{\frac{1}{3}}}, a\otimes a\right\rangle \geqslant 1$$

is in general not true (consider $F_n = \operatorname{diag}(n, 1, \frac{1}{n})$), whereas

$$\left\langle \frac{C}{(\det C)^{\frac{1}{3}}}, \mathbb{1}\right\rangle \geqslant 3$$

holds by virtue of Lemma A.11. □

**Lemma C.9** (Non-elliptic terms III). *Let $F \in \mathbb{M}^{3\times 3}$ and $M = a\otimes a$ with $\|a\| = 1$. Then the following terms are non-elliptic, hence non-quasiconvex*:

1. $F \mapsto W(F) = c_1 \operatorname{tr}(CM) - c_2 \ln\sqrt{\operatorname{tr}(CM)}.$
2. $F \mapsto W(F) = c_1 \operatorname{tr}(\operatorname{Adj} CM) - c_2 \ln\sqrt{\operatorname{tr}(\operatorname{Adj} CM)}.$

*with $c_1$, $c_2 > 0$. Observe that these terms have a physically desired singularity in fiber direction, i.e.*

$$W_S(F) \to \infty \quad \textit{as } F.a \to 0$$
$$W_S(F) \to \infty \quad \textit{as } \operatorname{Adj} F.a \to 0.$$

**Proof.** We show that the ellipticity condition is in general violated for the first term. We calculate

$$W_S(F) = c_1 \operatorname{tr}(CM) - c_2 \ln\sqrt{\operatorname{tr}(CM)} = c_1\|F.a\|^2 - c_2 \ln\|F.a\| = c_1\|F.a\|^2 - \frac{c_2}{2}\ln\|F.a\|^2.$$

Then calculating the first and second differential yields

$$DW_S(F).H = 2c_1\langle F.a, H.a\rangle - \frac{c_2}{\|F.a\|^2}\langle F.a, H.a\rangle$$
$$D^2W_S(F).(H,H) = 2c_1\|H.a\|^2 - c_2\left(\frac{1}{\|F.a\|^2}\|H.a\|^2 - 2\frac{\langle F.a, H.a\rangle^2}{\|F.a\|^4}\right).$$

Take $H = \xi \otimes \eta$ with $\|\xi\| = \|\eta\| = 1$. This gives

$$D^2 W_S(F).(\xi \otimes \eta, \xi \otimes \eta) = 2c_1 \|\xi\langle \eta, a\rangle\|^2 - c_2 \left( \frac{1}{\|F.a\|^2} \|\xi\langle \eta, a\rangle\|^2 - 2 \frac{\langle F.a, \xi\langle \eta, a\rangle^2\rangle}{\|F.a\|^4} \right)$$
$$= 2c_1 \langle \eta, a\rangle^2 - c_2 \left( \frac{\langle \eta, a\rangle^2}{\|F.a\|^2} - 2 \frac{\langle F.a, \xi\rangle\langle \eta, a\rangle^2}{\|F.a\|^4} \right).$$

Without loss of generality assume that $\xi$ is chosen such that $\langle F.a, \xi\rangle = 0$. It follows that

$$D^2 W_S(F).(\xi \otimes \eta, \xi \otimes \eta) = \langle \eta, a\rangle^2 \left( 2c_1 - \frac{c_2}{\|F.a\|^2} \right).$$

If the deformation $F$ in fiber direction $a$ is such that $\|F.a\|^2 < (c_2/2c_1)$ then

$$D^2 W_S(F).(\xi \otimes \eta, \xi \otimes \eta) = \langle \eta, a\rangle^2 \left( 2c_1 - \frac{c_2}{\|F.a\|^2} \right) < 0.$$

Observe that the more severe the deformation in fiber direction is, the more the ellipticity condition is violated. It is thus just the physically interesting region $\|F.a\|$ small which fails to be elliptic. Now we consider the second term. We calculate

$$W_S(F) = c_1 \operatorname{tr}(\operatorname{Adj} CM) - c_2 \ln \sqrt{\operatorname{tr}(\operatorname{Adj} CM)} = c_1 \|\operatorname{Adj} F^{\mathrm{T}}.a\|^2 - \frac{c_2}{2} \ln \|\operatorname{Adj} F^{\mathrm{T}}.a\|^2$$

$$DW_S(F).H = 2c_1 \langle \operatorname{Adj} F^{\mathrm{T}}.a, D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle - \frac{c_2}{\|\operatorname{Adj} F^{\mathrm{T}}.a\|^2} \langle \operatorname{Adj} F^{\mathrm{T}}.a, D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle$$

$$D^2 W_S(F).(H,H) = 2c_1 [\langle D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a, D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle + \langle \operatorname{Adj} F^{\mathrm{T}}.a, D^2\operatorname{Adj} F^{\mathrm{T}}.(H^{\mathrm{T}}, H^{\mathrm{T}}).a\rangle]$$
$$- \frac{c_2}{\|\operatorname{Adj} F^{\mathrm{T}}.a\|^2} [\langle D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a, D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle$$
$$+ \langle \operatorname{Adj} F^{\mathrm{T}}.a, D^2\operatorname{Adj} F^{\mathrm{T}}.(H^{\mathrm{T}}, H^{\mathrm{T}}).a\rangle]$$
$$+ \frac{2c_2}{\|\operatorname{Adj} F^{\mathrm{T}}.a\|^4} \langle \operatorname{Adj} F^{\mathrm{T}}.a, D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle^2.$$

Since $D^2\operatorname{Adj}F.(H,H) = 2\operatorname{Adj}H$ and for $H = \xi \otimes \eta$ we have $\operatorname{Adj}\xi \otimes \eta = 0$, it follows that

$$D^2 W_S(F).(\xi \otimes \eta, \xi \otimes \eta) = 2c_1 \|D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\|^2 - \frac{c_2}{\|\operatorname{Adj} F^{\mathrm{T}}.a\|^2} \|D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\|^2$$
$$+ \frac{2c_2}{\|\operatorname{Adj} F^{\mathrm{T}}.a\|^4} \langle \operatorname{Adj} F^{\mathrm{T}}.a, D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle^2$$
$$= \|D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\|^2 \left[ 2c_1 - \frac{c_2}{\|\operatorname{Adj} F^{\mathrm{T}}.a\|^2} \right]$$
$$+ \frac{2c_2}{\|\operatorname{Adj} F^{\mathrm{T}}.a\|^4} \langle \operatorname{Adj} F^{\mathrm{T}}.a, D\operatorname{Adj} F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle^2.$$

Consider $\langle \mathrm{Adj}\, F^{\mathrm{T}}.a, D\,\mathrm{Adj}\, F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle$. If we choose $F^{-T}.a = s\xi$ with $s \in \mathbb{R}^{+}$, then

$$\begin{aligned}
\langle \mathrm{Adj}\, F^{\mathrm{T}}.a, D\,\mathrm{Adj}\, F^{\mathrm{T}}.H^{\mathrm{T}}.a\rangle &= \langle \det F F^{-T}.a, \mathrm{Adj}\, F^{\mathrm{T}}[\langle F^{-1}, H^{\mathrm{T}}\rangle \mathbb{1} - H^{\mathrm{T}}F^{-T}].a\rangle \\
&= \det F^2 \langle F^{-T}.a, F^{-T}[\langle F^{-1}, \eta\otimes\xi\rangle \mathbb{1} - (\eta\otimes\xi)F^{-T}].a\rangle \\
&= \det F^2 \langle F^{-T}.a, \langle F^{-T}.\eta, \xi\rangle F^{-T}.a - F^{-T}.(\eta\otimes\xi)F^{-T}.a\rangle \\
&= \det F^2 \left[\|F^{-T}.a\|^2 \langle F^{-T}.\eta, \xi\rangle - \langle F^{-T}.a, F^{-T}.(\eta\otimes\xi)F^{-T}.a\rangle\right] \\
&= \det F^2 s^2 \left[\|\xi\|^2 \langle F^{-T}.\eta, \xi\rangle - \langle \xi, (F^{-T}.\eta\otimes\xi).\xi\rangle\right] \\
&= \det F^2 s^2 \left[1\langle F^{-1}.\xi, \eta\rangle - \langle \eta, F^{-1}.\xi 1\rangle\right] = 0.
\end{aligned}$$

With this choice we get

$$\begin{aligned}
D^2 W_S(F).(\xi\otimes\eta, \xi\otimes\eta) &= \|D\,\mathrm{Adj}\, F^{\mathrm{T}}.H^{\mathrm{T}}.a\|^2 \left[2c_1 - \frac{c_2}{\|\mathrm{Adj}\, F^{\mathrm{T}}.a\|^2}\right] \\
&= \|D\,\mathrm{Adj}\, F^{\mathrm{T}}.H^{\mathrm{T}}.a\|^2 \left[2c_1 - \frac{c_2}{\det F^2 \|F^{-T}.a\|^2}\right] \\
&= \|D\,\mathrm{Adj}\, F^{\mathrm{T}}.H^{\mathrm{T}}.a\|^2 \left[2c_1 - \frac{c_2}{\det F^2 s^2}\right].
\end{aligned}$$

Since $F$ can still be chosen with $\det F = 1$ taking $s > 0$ sufficiently small finishes the argument. □

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