Chapter 3

3.1 Representation of the free energy function

In the last tutorials, we showed two properties of the free energy function $\widehat{W}(\mathbb{F})$ based on two classes of transformations:

- **Material frame indifference** related to *change of observer in the actual configuration*:

$$\widehat{W}(\mathbb{F}) = \widehat{W}(\mathbf{Q}\mathbb{F}) \qquad \forall \mathbf{Q} \in \text{orth} \tag{3.1.1}$$

- **Material symmetry** related to *changes of reference configuration than do not affect the response of the material*:

$$\widehat{W}(\mathbb{F}) = \widehat{W}(\mathbb{F}\mathbb{P}) \qquad \forall \mathbb{P} \in \mathcal{G}_W \ , \tag{3.1.2}$$

where $\mathcal{G}_W$ is the *symmetry group* of the function $\widehat{W}$.

Note about the symmetry groups

- Biggest symmetry group, is the so called *unimodular group* unim $:= \{\mathbb{P} \in \mathbb{R}^{3\times 3}, |\det\mathbb{P}|=1\}$. Why cannot there be any bigger group? From the group property of the symmetry class, we know (by induction) that

$$\mathbb{P} \in \mathcal{G} \Longrightarrow \mathbb{P}^n \in \mathcal{G} \qquad \forall n \in \mathbb{N} \ .$$

Let us assume that some $\mathbb{P}_0$ such that $|\det\mathbb{P}_0| \neq 1$ would belong to $\mathcal{G}$, consequently it would have to hold

$$\widehat{W}(\mathbb{F}) = \widehat{W}(\mathbb{F}\mathbb{P}_0^n) \qquad \forall n \in \mathbb{N} \ , \tag{3.1.3}$$

which implies

$$\widehat{W}(\mathbb{F}) = \lim_{n\to\infty} \widehat{W}(\mathbb{F}\mathbb{P}_0^n) \ . \tag{3.1.4}$$

But

$$\lim_{n\to\infty} |\det\mathbb{P}_0^n| = \begin{cases} +\infty & \text{if} \quad |\det\mathbb{P}_0| > 1 \\ 0 & \text{if} \quad |\det\mathbb{P}_0| < 1 \end{cases} \tag{3.1.5}$$

Eq. (3.1.4) would then imply that energy of the material does not change if it is either infinitely expanded or, conversely, shrunk to a point. This clearly cannot be true. Which materials have this largest possible symmetry group? Fluids. (At least that is one way how to define what a fluid is.)

- Isotropic solids - the biggest symmetry group for solids is the orthogonal group

$$\text{orth} := \{\mathbb{P} \in \mathrm{R}^{3\times 3}, \mathbb{P}\mathbb{P}^T = \mathbb{P}^T\mathbb{P} = \mathbb{I}\} \subset \text{unim} \ . \tag{3.1.6}$$

Clearly orth is a proper subgroup of unim and it can be shown (see Noll, 1965) that it is a *maximal* proper subgroup of unimodular group, i.e. there is no group "between" the two. In other words, *there are only two classes of isotropic materials - either isotropic solids (symmetry group* = orth*) and fluids (symmetry group* = unim*).*

Isotropic hyperelastic solids

If we consider a class of hypereleastic solid materials with the maximal symmetry group, i.e. isotropic, we obtain by combining (3.1.1) and (3.1.2) with (3.1.6) (and replacing symbol $\mathbb{P}$ by $\mathbf{Q}$) that the free energy function of such materials must satisfy

$$\boxed{\widehat{W}(\mathbb{F}) = \widehat{W}(\mathbf{Q}\mathbb{F}) = \widehat{W}(\mathbb{F}\mathbf{Q}) \qquad \forall \mathbf{Q} \in \text{orth}} \,. \tag{3.1.7}$$

Exercise 1. Derive representation of $\widehat{W}(\mathbb{F})$ in terms of $\mathbb{C}$ and $\mathbb{B}$ show implications for the representations which follow from 3.1.7.
Solution: We employ the polar decomposition theorem

$$\mathbb{F} = \mathbb{V}\mathbf{R} = \mathbf{R}\mathbb{U}\,, \tag{3.1.8}$$

where $\mathbb{U}$ and $\mathbb{V}$ are symmetric, positive definite matrices and $\mathbf{R} \in$ orth.

Now we can proceed in two ways.

1. First employ material frame indifference and then symmetry (isotropy): Using $\mathbf{Q} = \mathbf{R}^T$ in the assumption of material frame indifference of free energy yields

$$\widehat{W}(\mathbb{F}) = \widehat{W}(\mathbf{R}^T\mathbf{R}\mathbb{U}) = \widehat{W}(\mathbb{U}) \;= \widetilde{W}(\mathbb{C})\,, \tag{3.1.9}$$

where, for convenience, we replaced $\mathbb{U}$ by the right Cauchy-Green deformation tensor $\mathbb{C} = \mathbb{F}^T\mathbb{F} = \mathbb{U}^T\mathbf{R}^T\mathbf{R}\mathbb{U} = \mathbb{U}^2$ and introduced a new function $\widetilde{W}(\mathbb{C}) = \widehat{W}(\mathbb{U})$. Now the implication of material symmetry for this new function gives for any $\mathbf{Q} \in$ orth:

$$\widetilde{W}(\mathbb{C}) = \widehat{W}(\mathbb{U}) = \widehat{W}(\mathbb{F}) = \widehat{W}(\mathbb{F}\mathbf{Q}) = \widetilde{W}(\mathbf{Q}\mathbb{C}\mathbf{Q}^T)\,, \tag{3.1.10}$$

or to summarize:

$$\boxed{\widetilde{W}(\mathbb{C}) = \widetilde{W}(\mathbf{Q}\mathbb{C}\mathbf{Q}^T) \qquad \forall \mathbf{Q} \in \text{orth}\,.} \tag{3.1.11}$$

This means, however, that the new function $\widetilde{W}(\mathbb{C})$ is **an isotropic scalar function** (see the general definition 1 below) of one tensorial argument in the sense of definition introduced last time.

2. First employ symmetry (isotropy) and then material frame indifference. Using $\mathbf{Q} = \mathbf{R}^T$ in the assumption of material symmetry (isotropy) yields

$$\widehat{W}(\mathbb{F}) = \widehat{W}(\mathbb{V}\mathbf{R}\mathbf{R}^T) = \widehat{W}(\mathbb{V}) \;= \overline{W}(\mathbb{B})\,, \tag{3.1.12}$$

where, for convenience, we replaced $\mathbb{V}$ by the left Cauchy-Green deformation tensor $\mathbb{B} = \mathbb{F}\mathbb{F}^T = \mathbb{V}\mathbf{R}\mathbf{R}^T\mathbb{V}^T = \mathbb{V}^2$ and introduced a new function $\overline{W}(\mathbb{B}) = \widehat{W}(\mathbb{V})$. Now the implication of material frame indifference for this new function gives for any $\mathbf{Q} \in$ orth:

$$\overline{W}(\mathbb{B}) = \widehat{W}(\mathbb{V}) = \widehat{W}(\mathbb{F}) = \widehat{W}(\mathbf{Q}\mathbb{F}) = \overline{W}(\mathbf{Q}\mathbb{B}\mathbf{Q}^T)\,, \tag{3.1.13}$$

or, to summarize:

$$\boxed{\overline{W}(\mathbb{B}) = \overline{W}(\mathbf{Q}\mathbb{B}\mathbf{Q}^T) \qquad \forall \mathbf{Q} \in \text{orth}\,.} \tag{3.1.14}$$

This means, however, that the new function $\overline{W}(\mathbb{B})$ is also **an isotropic scalar function** of one tensorial argument.

For the sake of completeness, let us give a more general definition of isotropic functions:

Definition 1 (Isotropic functions). We say that a scalar function $\widehat{a}$, vector function $\widehat{\mathbf{a}}$ and (symmetric) tensorial function $\widehat{\mathbb{A}}$, depending on scalar variables y_α, vectorial variables $\mathbf{y}_\alpha$ and symmetric tensorial variables $\mathbb{Y}_\alpha$, $\alpha = 1,\dots,N$ are called **isotropic**, if and only if

$$\widehat{a}(y_\alpha, \mathbf{y}_\alpha, \mathbb{Y}_\alpha) = \widehat{a}(y_\alpha, \mathbf{Q}\mathbf{y}_\alpha, \mathbf{Q}\mathbb{Y}_\alpha\mathbf{Q}^T) \qquad \forall \mathbf{Q} \in \text{orth}\,, \tag{3.1.15}$$

$$\mathbf{Q}\widehat{\mathbf{a}}(y_\alpha, \mathbf{y}_\alpha, \mathbb{Y}_\alpha) = \widehat{\mathbf{a}}(y_\alpha, \mathbf{Q}\mathbf{y}_\alpha, \mathbf{Q}\mathbb{Y}_\alpha\mathbf{Q}^T) \qquad \forall \mathbf{Q} \in \text{orth}\,, \tag{3.1.16}$$

$$\mathbf{Q}\widehat{\mathbb{A}}(y_\alpha, \mathbf{y}_\alpha, \mathbb{Y}_\alpha)\mathbf{Q}^T = \widehat{\mathbb{A}}(y_\alpha, \mathbf{Q}\mathbf{y}_\alpha, \mathbf{Q}\mathbb{Y}_\alpha\mathbf{Q}^T) \qquad \forall \mathbf{Q} \in \text{orth}\,. \tag{3.1.17}$$

So we just learned that for isotropic hyperelastic solids, we can represent the free energy function $\widehat{W}(\mathbb{F})$ in terms of two functions $\widetilde{W}(\mathbb{C})$ or $\overline{W}(\mathbb{B})$, both of which are isotropic functions. Why is this important? Because these functions have representation. In particular, the following holds

Theorem 3.1.1. *Representation theorem for a scalar isotropic function of 1 symmetric tensorial argument: Let $\psi(\mathbb{A}):\mathbb{R}^{3\times 3}_{\text{sym}}\to\mathbb{R}$ be isotropic, i.e.*

$$\psi(\mathbb{A})=\psi(\mathbf{Q}\mathbb{A}\mathbf{Q}^T)\qquad \forall\mathbf{Q}\in\text{orth}\ , \tag{3.1.18}$$

then

$$\psi(\mathbb{A})=\hat{\psi}(I_1(\mathbb{A}),I_2(\mathbb{A}),I_3(\mathbb{A}))\ , \tag{3.1.19}$$

where $I_i(\mathbb{A})$ i=1,2,3 are the principal invariants of $\mathbb{A}$:

$$I_1(\mathbb{A})=\text{tr}\mathbb{A}\ , \tag{3.1.20}$$

$$I_2(\mathbb{A})=\frac{1}{2}((\text{tr}\mathbb{A})^2-\text{tr}(\mathbb{A}^2)), \tag{3.1.21}$$

$$I_3(\mathbb{A})=\det\mathbb{A}\ . \tag{3.1.22}$$

So in view of what we've just learned about $\widetilde{W}(\mathbb{C})$ and $\overline{W}(\mathbb{B})$, we get the following representation of *free energy of an isotropic hyperelastic material*:

$$W=\widehat{W}(\mathbb{F})=\widetilde{W}(I_1(\mathbb{C}),I_2(\mathbb{C}),I_3(\mathbb{C}))=\overline{W}(I_1(\mathbb{B}),I_2(\mathbb{B}),I_3(\mathbb{B}))\ . \tag{3.1.23}$$

Exercise 2. Show, that the two above functions $\widetilde{W}(I_1(\mathbb{C}),I_2(\mathbb{C}),I_3(\mathbb{C}))$ and $\overline{W}(I_1(\mathbb{B}),I_2(\mathbb{B}),I_3(\mathbb{B}))$ are the same. Solution: The key is to realize, that the principal invariants of $\mathbb{C}$ and $\mathbb{B}$ are the same. This follows again from the polar decomposition:

$$\mathbb{C}=\mathbb{F}^T\mathbb{F}=(\mathbb{V}\mathbf{R})^T(\mathbb{V}\mathbf{R})=\mathbf{R}^T\mathbb{V}^2\mathbf{R}=\mathbf{R}^T\mathbb{B}\mathbf{R}\ , \tag{3.1.24}$$

where $\mathbf{R}\in$ orth, from where the statement follows. So we can write simply

$$W=\widehat{W}(\mathbb{F})=\hat{W}(I_i(\mathbb{C}))=\hat{W}(I_i(\mathbb{B}))\qquad i=1,2,3\ . \tag{3.1.25}$$

Having a representation of the free energy function is a very strong tool. Now we can easily prove representation of the three stress measures we know.:

Exercise 3 (Homework).

1. Show that for an isotropic hyperelastic material the following relationships hold that define the $\mathbb{T}$ - Cauchy stress tensor, $\hat{\mathbb{T}}^{(1)}$ - 1st Piola-Kirchhoff stress tensor and $\hat{\mathbb{T}}^{(2)}$ - 2nd Piola-Kirchhoff stress tensor:

$$\hat{\mathbb{T}}^{(1)}=2\mathbb{F}\frac{\partial\hat{W}(I_i(\mathbb{C}))}{\partial\mathbb{C}}=2\frac{\partial\hat{W}(I_i(\mathbb{B}))}{\partial\mathbb{B}}\mathbb{F}\ ,$$

$$\mathbb{T}^{(2)}=2\frac{\partial\hat{W}(I_i(\mathbb{C}))}{\partial\mathbb{C}}=2\mathbb{F}^{-1}\frac{\partial\hat{W}(I_i(\mathbb{B}))}{\partial\mathbb{B}}\mathbb{F}$$

$$\mathbb{T}=\frac{2}{\sqrt{\det\mathbb{C}}}\mathbb{F}\frac{\partial\hat{W}(I_i(\mathbb{C}))}{\partial\mathbb{C}}\mathbb{F}^T=\frac{2}{\sqrt{\det\mathbb{B}}}\frac{\partial\hat{W}(I_i(\mathbb{B}))}{\partial\mathbb{B}}\mathbb{B}$$

2. With the use of the above relations, prove that the Cauchy stress tensor of a hyperelastic isotropic solid has the following form:

$$\boxed{\mathbb{T}=a_0(I_i(\mathbb{B}))\,\mathbb{I}+a_1(I_i(\mathbb{B}))\,\mathbb{B}+a_2(I_i(\mathbb{B}))\,\mathbb{B}^2}\ , \tag{3.1.26}$$

where a_α α=0,1,2 are scalar functions of the principal invariants $I_i(\mathbb{B})$ ($i=1,2,3$).

Note: The last expression can be obtained also from the infamous Rivlin-Ericksen representation theorem. Let us give the statement here:

Theorem 3.1.2 (Rivlin-Ericksen)**.** *Let $\widehat{\mathbb{A}}$ by a symmetric tensorial (2nd order) function of one symmetric tensorial argument $\mathbb{Y}$. Then it is isotropic, i.e. it holds*

$$\boxed{\widehat{\mathbb{A}}(\mathbf{Q}\mathbb{Y}\mathbf{Q}^T) = \mathbf{Q}\widehat{\mathbb{A}}(\mathbb{Y})\mathbf{Q}^T}, \tag{3.1.27}$$

if and only if $\widehat{\mathbb{A}}$ is of the following form

$$\widehat{\mathbb{A}}(\mathbb{Y}) = a_0\mathbb{I} + a_1\mathbb{Y} + a_2\mathbb{Y}^2, \tag{3.1.28}$$

where

$$a_i = \hat{a}_i(I_1(\mathbb{Y}), I_2(\mathbb{Y}), I_3(\mathbb{Y})), \quad i = 1,2,3. \tag{3.1.29}$$

are functions of the principal invariants of $\mathbb{Y}$.

Note: We were able to prove Rivlin-Ericksen representation theorem for isotropic hyperelastic solids, as a result of the representation theorem for the free energy function. Realize that you have met R-E theorem already in the course on fluids, having the Cauchy stress $\mathbb{T}$ as a function of the symmetric velocity gradient $\mathbb{D}$, material frame indifference implies

$$\widehat{\mathbb{T}}(\mathbf{Q}\mathbb{D}\mathbf{Q}^T) = \mathbf{Q}\widehat{\mathbb{T}}(\mathbb{D})\mathbf{Q}^T, \tag{3.1.30}$$

which by R-E theorem yields a general representation of $\mathbb{T}$ in the form

$$\widehat{\mathbb{T}}(\mathbb{D}) = a_0\mathbb{I} + a_1\mathbb{D} + a_2\mathbb{D}^2, \tag{3.1.31}$$

where $a_i = \hat{a_i}(I_1(\mathbb{D}), I_2(\mathbb{D}), I_3(\mathbb{D}))$.

3.1.1 Representation in terms of principal stretches

Let us examine one more way of representing the free energy function of hyperelastic materials, which is widely used in literature to characterize particular real-world materials. This representation is based on replacing the principal invariants of $\mathbb{B}$ or $\mathbb{C}$ by eigenvalues of $\mathbb{B}$ and $\mathbb{C}$, or even more often, by their square roots - so called principal stretches. This leads to a representation

$$W = \hat{W}(\lambda_1, \lambda_2, \lambda_3), \tag{3.1.32}$$

where

$$\mathbb{C} = \sum_{i=1}^{3} \lambda_i^2 \mathbf{g}_i^{\mathbb{C}} \otimes \mathbf{g}_i^{\mathbb{C}}, \tag{3.1.33}$$

$$\mathbb{B} = \sum_{i=1}^{3} \lambda_i^2 \mathbf{g}_i^{\mathbb{B}} \otimes \mathbf{g}_i^{\mathbb{B}}, \tag{3.1.34}$$

with $\mathbf{g}_i^{\mathbb{C}}$ and $\mathbf{g}_i^{\mathbb{B}}$ being the normalized eigenvectors of $\mathbb{C}$ and $\mathbb{B}$, respectively. Such representation is in accord with the general form, since we know how to express the principal invariants of symmetric tensors in terms of eigenvalues $\omega_i = \lambda_i^2$:

$$I_1(\mathbb{B}) = I_1(\mathbb{C}) = \omega_1 + \omega_2 + \omega_3, \tag{3.1.35}$$

$$I_2(\mathbb{B}) = I_2(\mathbb{C}) = \omega_1\omega_2 + \omega_1\omega_3 + \omega_2\omega_3, \tag{3.1.36}$$

$$I_3(\mathbb{B}) = I_3(\mathbb{C}) = \omega_1\omega_2\omega_3, \tag{3.1.37}$$

so using the above relations together with $\omega_i = \lambda_i^2$ in representation (3.1.25) yields indeed representation (3.1.32). As far as the representation of the free energy is concerned, we are therefore done. It remains to clarify, how such a choice affects the expressions for stress measures. Looking at formulas, which you derived in the last homework, it is clear that we will have to be able to evaluate terms such as

$$\frac{\partial W}{\partial \mathbb{B}} = \sum_j \frac{\partial \tilde{W}(\lambda_1, \lambda_2, \lambda_3)}{\partial \lambda_j} \frac{\partial \lambda_j}{\partial \mathbb{B}} ,$$

or similarly with $\mathbb{C}$. The key point is the second part of the expression, the term $\frac{\partial \lambda_j(\mathbb{B})}{\partial \mathbb{B}}$, i.e. dependence of the (square root of) eigenvalue on the matrix.

Exercise 4. Derive the following identity

$$\boxed{\frac{\partial \lambda_\alpha(\mathbb{B})}{\partial \mathbb{B}} = \frac{1}{2\lambda_\alpha(\mathbb{B})} \mathbf{g}_\alpha^{\mathbb{B}} \otimes \mathbf{g}_\alpha^{\mathbb{B}}} \quad \text{(no summation)} . \tag{3.1.38}$$

Solution: Consider a smooth curve in the space of symmetric matrices, i.e. mapping $s \to \mathbb{B}(s)$: $\mathbb{R} \to \mathbb{R}^{3\times 3}_{\text{sym}}$ and let us replace for the moment λ_i^2 by ω_i. Along the curve, it holds (spectral decomposition)

$$\mathbb{B}(s) = \sum_{\alpha=1}^{3} \omega_\alpha(s) \mathbf{g}_\alpha^{\mathbb{B}}(s) \otimes \mathbf{g}_\alpha^{\mathbb{B}}(s) , \tag{3.1.39}$$

where both the eigenvalues ω_α and the eigenvectors $\mathbf{g}_\alpha^{\mathbb{B}}$ depend on the position on the curve. By orthonormality of $\{\mathbf{g}_\alpha^{\mathbb{B}}\}_{\alpha=1}^3$, we can express the eigenvalues on the curve as follows

$$\omega_\alpha(s) = \mathbf{g}_\alpha^{\mathbb{B}}(s) \cdot \mathbb{B}(s)\, \mathbf{g}_\alpha^{\mathbb{B}}(s) \quad \text{(no summation)}. \tag{3.1.40}$$

Let us take a tangent derivative, i.e. compute

$$\frac{d\omega(s)}{ds} = \mathbf{g}_\alpha^{\mathbb{B}}(s) \cdot \frac{d\mathbb{B}(s)}{ds} \mathbf{g}_\alpha^{\mathbb{B}}(s) + \frac{d\mathbf{g}_\alpha^{\mathbb{B}}(s)}{ds} \cdot \mathbb{B}(s) \mathbf{g}_\alpha^{\mathbb{B}}(s) + \mathbf{g}_\alpha^{\mathbb{B}}(s) \cdot \mathbb{B}(s) \frac{d\mathbf{g}_\alpha^{\mathbb{B}}(s)}{ds} . \tag{3.1.41}$$

The last two terms are zero, since

$$\frac{d\mathbf{g}_\alpha^{\mathbb{B}}(s)}{ds} \cdot \mathbb{B}(s) \mathbf{g}_\alpha^{\mathbb{B}}(s) = \omega_\alpha(s) \frac{d\mathbf{g}_\alpha^{\mathbb{B}}(s)}{ds} \cdot \mathbf{g}_\alpha^{\mathbb{B}}(s) = \omega_\alpha(s) \frac{d}{ds} \underbrace{(\mathbf{g}_\alpha^{\mathbb{B}}(s) \cdot \mathbf{g}_\alpha^{\mathbb{B}}(s))}_{\equiv 1} = 0 , \tag{3.1.42}$$

and

$$\mathbf{g}_\alpha^{\mathbb{B}}(s) \cdot \mathbb{B}(s) \frac{d\mathbf{g}_\alpha^{\mathbb{B}}(s)}{ds} = (\mathbb{B}(s) \mathbf{g}_\alpha^{\mathbb{B}}(s)) \cdot \frac{d\mathbf{g}_\alpha^{\mathbb{B}}(s)}{ds} = 0 , \tag{3.1.43}$$

by the same argument, thanks to symmetry of $\mathbb{B}$. So we got

$$\frac{d\omega(s)}{ds} = \mathbf{g}_\alpha^{\mathbb{B}}(s) \cdot \frac{d\mathbb{B}(s)}{ds} \mathbf{g}_\alpha^{\mathbb{B}}(s) = (\mathbf{g}_\alpha^{\mathbb{B}}(s) \otimes \mathbf{g}_\alpha^{\mathbb{B}}(s)) : \frac{d\mathbb{B}(s)}{ds} \quad \text{(no summation)}. \tag{3.1.44}$$

The left-hand side equivalently reads by chain-rule

$$\frac{d\omega(s)}{ds} = \frac{d\omega(\mathbb{B}(s))}{ds} = \frac{d\omega(\mathbb{B}(s))}{d\mathbb{B}} : \frac{d\mathbb{B}(s)}{ds} . \tag{3.1.45}$$

Comparing the two expressions, and realizing that it must hold for arbitrary (smooth) curve (i.e. arbitrary tangent $\frac{d\mathbb{B}(s)}{ds}$), yields finally

$$\frac{d\omega_\alpha(\mathbb{B})}{d\mathbb{B}} = \mathbf{g}_\alpha^{\mathbb{B}} \otimes \mathbf{g}_\alpha^{\mathbb{B}} \quad \text{(no summation)} . \tag{3.1.46}$$

Using finally $\omega_\alpha(\mathbb{B}) = \lambda_\alpha^2(\mathbb{B})$ yields the desired expression.

Exercise 5. Homework Consider so-called **compressible Ogden material**, a model of an isotropic hyperelastic material, which well describes most rubber-like materials. The free energy of compressible Ogden material is often written as follows

$$W(\lambda_1, \lambda_2, \lambda_3) = \sum_{k=1}^{N} \frac{\mu_k}{\alpha_k} \left(\lambda_1^{\alpha_k} + \lambda_2^{\alpha_k} + \lambda_3^{\alpha_k} - 3\right) , \tag{3.1.47}$$

where α_k are real constants and μ_k are (constant) shear moduli. Using the above exercise, derive the form of Cauchy stress tensor for compressible Ogden material.