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# GENERIC for dissipative solids with bulk-interface interaction

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# GENERIC for dissipative solids with bulk-interface interaction

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**Abstract**

The modeling framework of GENERIC was originally introduced by Grmela and Öttinger for thermodynamically closed systems. It is phrased with the aid of the energy and entropy as driving functionals for reversible and dissipative processes and suitable geometric structures. Based on the definition functional derivatives we propose a GENERIC framework for systems with bulk-interface interaction and apply it to discuss the GENERIC structure of models for delamination processes.

## 1 Introduction

GENERIC, the acronym for General Equation of Non-Equilibrium Reversible Irreverslible Coupling, is a thermodynamical modeling framework originally introduced by Grmela and Öttinger in [GÖ97, ÖG97] for thermodynamically closed systems with applications in fluid dynamics. In recent years its versatility has been proved also for many other applications such as dissipative solids [Mie11a, HS12, Mie16], complex and reactive fluids [MBZ18, PTA$^+$19, ZPT21, VPE21], semiconductors and electro-chemistry [GM13, MPRT, MM20], quantum mechanics [MM17], and thermodynamical multiscale processes [PKG18]. A GENERIC system is characterized by a quintuple $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ consisting of a state space $\mathcal{Q}$, the two driving potentials: $\mathcal{E}$ the total energy and $\mathcal{S}$ the entropy, and two geometric structures: $\mathbb{J}$ a Poisson operator and $\mathbb{K}$ an Onsager operator. Herein, the triple $(\mathcal{Q}, \mathcal{E}, \mathbb{J})$ forms a Hamiltonian system characterizing the reversible contributions to the dynamics and the triple $(\mathcal{Q}, \mathcal{S}, \mathbb{K})$ forms an Onsager system accounting for the irreversible, dissipative contributions to dynamics. These two triples are coupled in a GENERIC system under an additional constraint, the so-called noninteraction condition NIC, stating that $\mathbb{K}\mathrm{D}\mathcal{E} \equiv 0 \equiv \mathbb{J}\mathrm{D}\mathcal{S}$. In thermodynamically closed systems the NIC automatically ensures conservation of energy and entropy production. The dynamics of the GENERIC system is then described by the evolution equation

$$\dot{q} = \mathbb{J}\mathrm{D}\mathcal{E}(q) + \mathbb{K}\mathrm{D}\mathcal{S}(q)\,,$$

which clearly displays the coupled evolution with reversible and dissipative contributions. The thermodynamical driving forces are the functional derivatives $\mathrm{D}\mathcal{E}(q)$ for reversible dynamics and $\mathrm{D}\mathcal{S}(q)$ for dissipative dynamics. In Section 2 we review the GENERIC framework for thermodynamically closed systems. It is the central aim of this work to extend the GENERIC framework to systems with bulk-interface interaction. These are systems composed of two (or more) subsystems $\Omega_\pm \subset \mathbb{R}^d$ coupled with each other along a joint interface $\Gamma \subset \mathbb{R}^{d-1}$ through which they exchange quantities like heat, stresses, mass, etc.. Along $\Gamma$ also additional processes may take place that are modeled by additional state variables solely defined on $\Gamma$ with individual evolution laws on $\Gamma$, but also driven by the interaction with the quantities from the bulk subdomains $\Omega_\pm$. While the compound $\Omega = \mathrm{int}\big(\overline{\Omega_+} \cup \overline{\Omega_-}\big)$ can be assumed to form a thermodynamically closed system, none of the two individual subsystems $\Omega_\pm$ nor the interface $\Gamma$ do so. Each of these components alone is an open system. A first approach to the

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GENERIC framework for thermodynamically open systems was made in [Ött06] using driving functionals and geometric structures for the bulk and the boundary components. Here we follow this idea and, based on the definition of functional derivatives for functionals with bulk and interfacial contributions given in Section 3.1, we propose in Section 3.3 to regard the GENERIC formulation for bulk-interface processes in terms of a weak formulation. We also study the properties of geometric structures for systems with bulk-interface interaction in Section 3.2. In order to ensure the NIC for GENERIC systems of dissipative solids it was developed in [Mie11a] for closed systems that this can be achieved with the aid of certain thermodynamic transformation maps. In Section 3.4 we show that this approach can also be applied to systems with bulk-interface interaction, again by exploiting the definition and structure of the funtional derivatives involved in this transformation. We subsequently demonstrate the versatility of the weak formulation of GENERIC in Section 4 for thermo-viscoelastic materials experiencing delamination processes along $\Gamma$. It is shown that the weak formulation of GENERIC leads to well-known bulk equations and naturally provides interfacial coupling conditions along $\Gamma$.

# 2 The GENERIC formalism for closed systems

Let $\mathcal{Q}$ be a Banach space and $\mathcal{V}$ a Hilbert space such that $\mathcal{Q} \hookrightarrow \mathcal{V} = \mathcal{V}^* \hookrightarrow \mathcal{Q}^*$ are dense. We denote for $q \in \mathcal{Q}$ and $q^* \in \mathcal{Q}^*$ the duality pairing by $\langle q^*, q\rangle_{\mathcal{Q}}$ and say that a linear operator $\mathbb{A} : \mathcal{Q}^* \to \mathcal{Q}$ is *symmetric*, resp. *antisymmetric* if for every $q_1^*, q_2^* \in \mathcal{Q}^*$ it holds

$$\langle q_1^*, \mathbb{A}q_2^*\rangle_{\mathcal{Q}} = \langle q_2^*, \mathbb{A}q_1^*\rangle_{\mathcal{Q}}\,, \quad \text{resp.} \quad \langle q_1^*, \mathbb{A}q_2^*\rangle_{\mathcal{Q}} = -\langle q_2^*, \mathbb{A}q_1^*\rangle_{\mathcal{Q}}\,.$$

In most parts of the computations below, the reader may think of the Hilbert case $\mathcal{Q} = \mathcal{V}$. In this case, the above definitions coincide with the classical definitions $\mathbb{A} = \mathbb{A}^*$ resp. $\mathbb{A} = -\mathbb{A}^*$. For a functional $\Phi : \mathcal{Q} \to \mathbb{R}$ we denote the

$$\text{Gâteaux derivative: } \delta\Phi : \mathcal{Q} \to \mathcal{Q}^*, \text{ i.e., the first variation,} \tag{1a}$$

$$\text{Fréchet derivative: } \mathrm{D}\Phi : \mathcal{Q} \to \mathcal{Q}^*\,, \tag{1b}$$

if they exist and we recall that $\mathrm{D}\Phi(q) = \delta\Phi(q)$ if $\mathrm{D}\Phi(q)$ exists. We finally define

$$\delta\Phi(q)[\tilde{q}] := \langle \delta\Phi(q), \tilde{q}\rangle_{\mathcal{Q}}\,, \qquad \mathrm{D}\Phi(q)[\tilde{q}] := \langle \mathrm{D}\Phi(q), \tilde{q}\rangle_{\mathcal{Q}}\,.$$

## 2.1 Hamiltonian systems $(\mathcal{Q}, \mathcal{E}, \mathbb{J})$

In the spirit of Hamiltonian mechanics, a general Hamiltonian system accounts for reversible dynamics, only. The equations of motion are given by

$$\dot{q} = \mathbb{J}\mathrm{D}\mathcal{E}(q) \in \mathcal{Q}\,. \tag{2}$$

The driving potential of reversible dynamics is the total energy functional of the system $\mathcal{E} : \mathcal{Q} \to \mathbb{R}$, which may comprise kinetic, mechanical, chemical, electric and thermal energy. The defining property for a Hamiltonian system is that the associated geometric structure $\mathbb{J}$ is a *Poisson structure*, i.e.

$$\mathbb{J} : \mathcal{Q}^* \to \mathcal{Q} \text{ is antisymmetric, and satisfies Jacobi's identity.} \tag{3}$$

More precisely, (3) ensures that the *Poisson bracket* $\{\cdot,\cdot\}$ defined by $\{\Phi_1, \Phi_2\} := \langle \mathrm{D}\Phi_1, \mathbb{J}\mathrm{D}\Phi_2\rangle_{\mathcal{Q}}$ for all $\Phi_j : \mathcal{Q} \to \mathbb{R}$ is an

$$\begin{aligned}&\text{antisymmetric bilinear form and satisfies Jacobi's identity, i.e.} \\ &\forall \Phi_1, \Phi_2, \Phi_3 : \mathcal{Q} \to \mathbb{R} : \quad \{\Phi_1, \{\Phi_2, \Phi_3\}\} + \{\Phi_3, \{\Phi_1, \Phi_2\}\} + \{\Phi_2, \{\Phi_3, \Phi_1\}\} = 0\,.\end{aligned} \tag{4}$$

Moreover, the Poisson bracket fulfills the Leibniz rule:

$$\{\Phi_1\Phi_2, \Phi_3\} = \Phi_1\{\Phi_2, \Phi_3\} + \{\Phi_1, \Phi_3\}\Phi_2 \text{ for all } \Phi_1, \Phi_2, \Phi_3 : \mathcal{Q} \to \mathbb{R}\,. \tag{5}$$

Conditions (4) and (5) are the defining properties of a *symplectic* structure, which is the geometric structure underlying Hamiltonian mechanics, see e.g. [AKN06, Sect. 1.3]. Let us also mention that the requirement of Jacobi's identity provides a generalization of the commutativity of derivatives. Indeed, for $\mathcal{Q} = \mathcal{Q}_1 \times \mathcal{Q}_2$ and $\mathbb{J}$ in canonical form, i.e., $\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$, it can be checked that fulfilling Jacobi's identity amounts to validity of $\mathrm{D}_{q_1}\mathrm{D}_{q_2}\Phi_i = \mathrm{D}_{q_2}\mathrm{D}_{q_1}\Phi_i$. See e.g. [ZPT21, D'A15, Mor98] for further discussion of Jacobi's identity.

The antisymmetry of $\mathbb{J}$ implies $\langle q', \mathbb{J}q'\rangle_{\mathcal{Q}} = -\langle q', \mathbb{J}q'\rangle_{\mathcal{Q}} = 0$ for any $q' \in \mathcal{Q}^*$ and conservation of energy along solutions of (2) follows immediately:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(q(t)) = \langle \mathrm{D}\mathcal{E}(q), \dot{q}\rangle_{\mathcal{Q}} = \langle \mathrm{D}\mathcal{E}(q), \mathbb{J}\mathrm{D}\mathcal{E}(q)\rangle_{\mathcal{Q}} = 0\,. \tag{6}$$

## 2.2 Onsager systems $(\mathcal{Q}, \mathcal{S}, \mathbb{K})$ (gradient systems)

An Onsager system is related to the dynamics of irreversible, dissipative effects. The evolution equations read

$$\dot{q} = \mathbb{K}(q)\mathrm{D}\mathcal{S}(q) \in \mathcal{Q}\,. \tag{7}$$

The driving functional is the total entropy $\mathcal{S}$ and the associated geometric structure is imposed by the so-called *Onsager operator* $\mathbb{K}$ with the properties:

$$\mathbb{K} \text{ is symmetric and positive semidefinite, i.e. } \langle \xi, \mathbb{K}\xi\rangle_{\mathcal{Q}} \geq 0\,. \tag{8}$$

The symmetry of $\mathbb{K}$ reflects the *Onsager principle*, which states that the *rate* equals the *symmetric, positively semidefinite operator* $\mathbb{K}$ applied to the *thermodynamically conjugate force*. The positive semidefiniteness is a manifestation of the second law of thermodynamics, i.e. we have an increase of entropy via

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(q(t)) = \langle \mathrm{D}\mathcal{S}(q), \dot{q}\rangle_{\mathcal{Q}} = \langle \mathrm{D}\mathcal{S}(q), \mathbb{K}\mathrm{D}\mathcal{S}\rangle_{\mathcal{Q}} \geq 0. \tag{9}$$

The properties of $\mathbb{K}$ are equivalent to the existence of a nonnegative, quadratic dual entropy-production (or dissipation) potential $\Psi^* = \Psi^*(q;\xi) = \frac{1}{2}\langle \xi, \mathbb{K}(q)\xi\rangle_{\mathcal{Q}}$, see [Mie11b]. This can be generalized to non-quadratic potentials as follows:

$$\text{For all } q \in \mathcal{Q},\ \Psi^*(q;\cdot) \text{ is nonnegative, convex, and } \Psi^*(q;0) = 0. \tag{10}$$

In particular, for all $q \in \mathcal{Q}$ the potential $\Psi^*$ is the convex conjugate of a nonnegative, convex dissipation potential $\Psi(q;\cdot) : \mathcal{Q} \to [0,\infty]$ with the property $\Psi^*(q;0) = 0$. The convex conjugate is defined by

$$\Psi^*(q;\xi) := \sup_{\tilde{q}\in\mathcal{Q}} \big(\langle \xi, \tilde{q}\rangle_{\mathcal{Q}} - \Psi(q;\tilde{q})\big) \quad \text{for all } (q,\xi) \in \mathcal{Q}\times\mathcal{Q}^*\,. \tag{11}$$

In this generalized setting, the evolution reads

$$\dot{q} \in \partial_\xi \Psi^*(q; \mathrm{D}\mathcal{S}(q)) \quad \text{in } \mathcal{Q}$$

with $\partial_\xi \Psi^*(q,\xi)$ the (multivalued) subdifferential of $\Psi^*(q,\cdot)$ in $\xi \in \mathcal{Q}^*$, i.e.,

$$\partial_\xi \Psi^*(q;\xi) = \{\tilde{q} \in \mathcal{Q},\ \Psi^*(q;\tilde{\xi}) - \Psi^*(q;\xi) \geq \langle \tilde{\xi} - \xi, \tilde{q}\rangle_{\mathcal{Q}} \text{ for all } \tilde{\xi} \in \mathcal{Q}^*\}\,. \tag{12}$$

We point to Section 3.2, where we discuss further implications of (10). Non-quadratic dual dissipation potentials arise, e.g., for generalized standard materials with a rate-independent evolution of the internal variable: Here, $\Psi^*(q,\cdot)$ is positively $1$-homogeneous. For further details we refer to Section 4 as well as to [Mie11a].

## 2.3 GENERIC systems $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$

A GENERIC system is a quintuple $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$, which couples a Hamiltonian system $(\mathcal{Q}, \mathcal{E}, \mathbb{J})$ with an Onsager system $(\mathcal{Q}, \mathcal{S}, \mathbb{K})$. The combined evolution equations have the form

$$\dot{q} = \mathbb{J}(q)\mathrm{D}\mathcal{E}(q) + \mathbb{K}(q)\mathrm{D}\mathcal{S}(q), \tag{13}$$

displaying the reversible and the irreversible part of the dynamics. Appart from the structural relations (3) and (8) of Hamiltonian and Onsager systems, a GENERIC system additionally has to satisfy the following crucial and nontrivial

$$\textbf{noninteraction condition, NIC:} \qquad \mathbb{K}\mathrm{D}\mathcal{E} \equiv 0 \qquad \text{and} \qquad \mathbb{J}\mathrm{D}\mathcal{S} \equiv 0\,. \tag{14}$$

If $\mathbb{K}$ arises from a (subdifferential of a) non-quadratic dual dissipation potential $\Psi^*(q;\cdot)$ as introduced in (10), then the NIC $\mathbb{K}\mathrm{D}\mathcal{E} = 0$ needs to be replaced by

$$\Psi^*(q;\xi + \lambda \mathrm{D}\mathcal{E}(q)) = \Psi^*(q;\xi) \ \text{ for all } q \in \mathcal{Q},\ \xi \in \mathcal{Q}^*, \text{ and } \lambda \in \mathbb{R}\,. \tag{15}$$

We refer to Sec. 3.2 and to [Mie11a, Sec. 2.5] for more details.

**Remark 2.1** (Direct consequences of NIC)**.** The NIC (14) ensures that the energy functional does not contribute to dissipative mechanisms and that the entropy functional does not contribute to reversible dynamics, i.e. every solution $q$ of (13) satisfies:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(q(t)) = \langle \mathrm{D}\mathcal{E}(q), \dot{q}\rangle = \langle \mathrm{D}\mathcal{E}(q), \mathbb{J}\mathrm{D}\mathcal{E} + \mathbb{K}\mathrm{D}\mathcal{S}\rangle = 0 + 0 = 0\,, \tag{16}$$

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{S}(q(t)) = \langle \mathrm{D}\mathcal{S}(q), \dot{q}\rangle = \langle \mathrm{D}\mathcal{S}(q), \mathbb{J}\mathrm{D}\mathcal{E} + \mathbb{K}\mathrm{D}\mathcal{S}\rangle = 0 + \langle \mathrm{D}\mathcal{S}, \mathbb{K}\mathrm{D}\mathcal{S}\rangle \geq 0\,, \tag{17}$$

Moreover, the NIC (14) guarantee the validity of the principle of maximum-entropy production. See e.g. [ZPT21, ÖG97, GÖ97, Mie11a] for more details. ⋆

# 3 GENERIC formalism for bulk-interface systems

Our investigations will be based on the following specific geometric setting:

**Definition 3.1** (Geometric setup and notation)**.** *Let $\Omega_+, \Omega_- \subset \mathbb{R}^d$ be the reference domains of two bodies with $\Omega_+ \cap \Omega_- = \emptyset$, let $\partial\Omega_\pm$ their boundaries with outer unit normal $\mathrm{n}_\pm$ and joint interface $\Gamma := \partial\Omega_+ \cap \partial\Omega_-$. For better clarification we further introduce the notation $\Gamma_\pm := \Gamma \cap \partial\Omega_\pm$, $\mathrm{B} := \Omega_+ \cup \Omega_-$ and $\Omega := \mathrm{int}(\overline{\Omega_+} \cup \overline{\Omega_-})$.*

*The geometric setup is described by one of the following two scenarios:*

1 *The two subdomains $\Omega_+$ and $\Omega_-$ are connected with each other along $\Gamma \neq \emptyset$. The domain $\Omega := \operatorname{int}(\overline{\Omega_+} \cup \overline{\Omega_-})$ is again thermodynamically closed. Hence, the only exchange that $\Omega_\pm$ has with its surroundings is that with $\Omega_\mp$ along $\Gamma$.*

2 *As a special case of 1., the subdomain $\Omega_+$ is surrounded by $\Omega_-$ so that $\Gamma = \partial\Omega_+$ and $\partial\Omega = \partial\Omega_- \backslash \Gamma$.*

*For a function $\phi : \Omega\backslash\Gamma \to \mathbb{R}$ we denote by $\phi_\pm = \phi|_{\Omega_\pm}$ its restriction to $\Omega_\pm$, by $\gamma_\pm\phi_\pm$ its trace from $\Omega_\pm$ onto $\partial\Omega_\pm$, and by $[\![\phi]\!] := (\gamma_+\phi_+ - \gamma_-\phi_-)$ its jump across $\Gamma$. Moreover, we use the short-hand notation $\phi_\gamma := (\gamma_+\phi_+, \gamma_-\phi_-)$ and if no confusion is possible, we abbreviate*

$$\gamma_\pm\phi_\pm = \gamma\phi_\pm = \phi_\pm \quad \textit{and} \quad \phi_\gamma = (\phi_+, \phi_-) \quad \textit{on}\ \Gamma\,. \tag{18}$$

*A similar notation is adopted for vector- and tensor-valued functions and has to be understood componentwise.*

## 3.1 Functional calculus for bulk-interface systems: Notation, differentials, and $*$-multiplication in the setup of Def. 3.1

**States and spaces.** In the setup of Def. 3.1 consider the function spaces $\mathcal{Q}_{\mathrm{B}} := \mathcal{Q}_+ \times \mathcal{Q}_-$ and $\mathcal{Q} = \mathcal{Q}_{\mathrm{B}} \times \mathcal{Q}_\Gamma$ with $\mathcal{Q}_\pm$ being a Banach space (e.g. a Sobolev space) defined on $\Omega_\pm$ and with $\mathcal{Q}_\Gamma$ being a Banach space defined on $\Gamma$ with dual spaces $\mathcal{Q}_\pm^*, \mathcal{Q}_{\mathrm{B}}, \mathcal{Q}_\Gamma^*$, and the dual pairings by $\langle\cdot,\cdot\rangle_{\mathcal{Q}_\pm}$, resp. $\langle\cdot,\cdot\rangle_{\mathcal{Q}_{\mathrm{B}}}$, $\langle\cdot,\cdot\rangle_{\mathcal{Q}_\Gamma}$. The states $q = (q_{\mathrm{B}}, q_\Gamma)$ are composed of bulk states $q_{\mathrm{B}} \in \mathcal{Q}_{\mathrm{B}}$ with $q_\pm := q_{\mathrm{B}}|_{\Omega_\pm}$ and surface states $q_\Gamma \in \mathcal{Q}_\Gamma$. Here, a surface state $q_\Gamma$ is supposed to have an own evolution equation on $\Gamma$ so that its evolution is not solely governed from the bulk. For shorter notation we also introduce the vector

$$q_{\Gamma\gamma} := (\gamma_+ q_+, \gamma_- q_-, q_\Gamma) \in \gamma\mathcal{Q}_{\mathrm{B}} \times \mathcal{Q}_\Gamma\,, \tag{19}$$

where $\gamma\mathcal{Q}_{\mathrm{B}}$ denotes the trace space corresponding to $\mathcal{Q}_{\mathrm{B}}$. More precisely, let the state $q = (q_{\mathrm{B}}, q_\Gamma) = (q_{\mathrm{B}_1}, \dots, q_{\mathrm{B}_l}, q_{\Gamma_1}, \dots, q_{\Gamma_m}) \in \mathcal{Q}$. If the state variable $q_{\mathrm{B}k}|_{\Omega_\pm}$ has a well-defined trace on $\Gamma$, then the $k$th component of $\gamma_\pm q_\pm$ in (19) is given by the trace $\gamma_\pm q_{k\pm}$. Instead, if the trace of this state variable does not exist, then we set the $k$th component of $\gamma_\pm q_\pm$ equal to zero in $q_{\Gamma\gamma}$. In this latter case, $\gamma_\pm\mathcal{Q}_{k\pm} = \{0\}$.

**Example 3.2** (Notation (19))**.** Consider a system with bulk states

$$q_{\mathrm{B}} = (q_{\mathrm{B}1}, q_{\mathrm{B}2}) = (q_{1+}, q_{2+}, q_{1-}, q_{2-})$$

and with one single interface state $q_{\Gamma 1}$. Assume $q_{1\pm}$ have well-defined traces on $\Gamma$, whereas $q_{2\pm}$ don't. Accordingly, $q_{\Gamma\gamma} = (\gamma_+ q_{1+}, 0, \gamma_- q_{1-}, 0, q_{\Gamma 1})$, where the entries $0$ substitute the (non-existing) traces of $q_{2\pm}$. ⋆

**Functionals and their derivatives.** Let $\Phi = \Phi_{\mathrm{B}} + \Phi_\Gamma : \mathcal{Q} \to \mathbb{R}$ denote an integral functional with density $\phi = (\phi_{\mathrm{B}}, \phi_\Gamma)$, which contains a bulk contribution $\phi_{\mathrm{B}}$ and a surface contribution $\phi_\Gamma$ on $\Gamma$, i.e., for all states $q \in \mathcal{Q}$ it is

$$\Phi(q) = \int_{\Omega\backslash\Gamma} \phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}})\,\mathrm{d}x + \int_\Gamma \phi_\Gamma(\gamma_+ q_+, \gamma_- q_-, q_\Gamma)\,\mathrm{d}\mathcal{H}^{d-1}\,. \tag{20}$$

Let again $q = (q_{\mathrm{B}}, q_\Gamma) = (q_{\mathrm{B}_1}, \dots, q_{\mathrm{B}_l}, q_{\Gamma_1}, \dots, q_{\Gamma_m}) = (q_j)_{j=1}^{l+m} \in \mathcal{Q} = \Pi_{j=1}^{l+m} \mathcal{Q}_j$, and $q_k$ the kth component in this vector. Restricting $\Phi$ to the affine space $\mathcal{Q}_k$, with $q_k \in \mathcal{Q}_k$, we use the following notation for the

$$\text{first variation wrt. } q_k: \quad \delta_{q_k}\Phi : \mathcal{Q} \to \mathcal{Q}_k^*, \tag{21a}$$

$$\text{functional derivative wrt. } q_k: \quad \mathrm{D}_{q_k}\Phi : \mathcal{Q} \to \mathcal{Q}_k^*, \tag{21b}$$

$$\text{partial derivative of a density } \phi = \phi(q) \text{ wrt. } q_k: \quad \partial_{q_k}\phi(q)\,. \tag{21c}$$

For $\Phi$ from (20) and a bulk state $q_k$ it is

$$\begin{aligned}\delta_{q_k}\Phi(q)[\tilde{q}_k] =& \delta_{q_k}\Phi_{\mathrm{B}}(q_{\mathrm{B}})[\tilde{q}_k] + \delta_{q_k}\Phi_\Gamma(q)[\tilde{q}_k] \\ =& \int_{\Omega\setminus\Gamma} \big(\partial_{q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}})\tilde{q}_k + \partial_{\nabla q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}}) \cdot \nabla\tilde{q}_k\big)\,\mathrm{d}x \\ &+ \sum_{i\in\{+,-\}} \int_\Gamma \partial_{q_{k_i}}\phi_\Gamma(\gamma_+ q_+, \gamma_- q_-, q_\Gamma)\gamma_{k_i}\tilde{q}_{k_i}\,\mathrm{d}\mathcal{H}^{d-1}\,, \end{aligned} \tag{21d}$$

$$\begin{aligned}\text{and } \mathrm{D}_{q_k}\Phi(q)[\tilde{q}_k] =& \mathrm{D}_{q_k}\Phi_{\mathrm{B}}(q_{\mathrm{B}})[\tilde{q}_k] + \mathrm{D}_{q_k}\Phi_\Gamma(q)[\tilde{q}_k] \\ =& \int_{\Omega\setminus\Gamma} \big(\partial_{q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}}) - \operatorname{div}\partial_{\nabla q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}})\big)\tilde{q}_k\,\mathrm{d}x \\ &+ \sum_{i\in\{+,-\}} \int_\Gamma \big(\partial_{\nabla q_k}\phi_{\mathrm{B}}(q_i, \nabla q_i)\cdot \mathrm{n}_i + \partial_{q_{k_i}}\phi_\Gamma(q_+, q_-, q_\Gamma)\big)\tilde{q}_{k_i}\,\mathrm{d}\mathcal{H}^{d-1}. \end{aligned} \tag{21e}$$

i.e., by integration by parts we have the equivalence

$$\delta_{q_k}\Phi(q)[\tilde{q}_k] = \mathrm{D}_{q_k}\Phi(q)[\tilde{q}_k]\,. \tag{21f}$$

Similarly, for $\Phi$ from (20) and a surface state $q_k$ it is

$$\begin{aligned}\delta_{q_k}\Phi(q)[\tilde{q}_k] &= \int_\Gamma \big(\partial_{q_k}\phi_\Gamma(\gamma_+ q_+, \gamma_- q_-, q_\Gamma)\tilde{q}_k + \partial_{q_{k_-}}\phi_\Gamma(q_+, q_-, q_\Gamma)\tilde{q}_{k_-}\big)\,\mathrm{d}\mathcal{H}^{d-1} \\ &= \mathrm{D}_{q_k}\Phi(q)[\tilde{q}_k]\,. \end{aligned} \tag{21g}$$

Given a sufficiently smooth function $\alpha : \Omega\setminus\Gamma \to \mathbb{R}$ we introduce the multiplication operation $*$ as follows

$$\begin{aligned}\alpha * \mathrm{D}_{q_k}\Phi(q)[\tilde{q}_k] =& \int_{\Omega\setminus\Gamma} \big(\alpha\partial_{q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}}) - \operatorname{div}\big(\alpha\partial_{\nabla q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}})\big)\big)\tilde{q}_k\,\mathrm{d}x \\ &+ \sum_{i\in\{+,-\}} \int_\Gamma \big(\alpha\partial_{q_{k_i}}\phi_\Gamma(q_+, q_-, q_\Gamma) + \alpha\partial_{\nabla q_k}\phi_{\mathrm{B}}(q_i, \nabla q_i)\cdot \mathrm{n}_i\big)\tilde{q}_{k_+}\,\mathrm{d}\mathcal{H}^{d-1}\,. \end{aligned} \tag{22}$$

We will use the above notation for differentials and $*$ multiplication also for densities $\phi$ themselves. Exemplarily we indicate this here for a bulk state $q_k$ :

$$\begin{aligned}\delta_{q_k}\phi(q)[\square] =& \left[\partial_{q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}})\square + \partial_{\nabla q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}})\cdot\nabla\square\right]_{\Omega\setminus\Gamma} \\ &+ \sum_{i\in\{+,-\}} \Big[\partial_{q_{k_i}}\phi_\Gamma(q_+, q_-, q_\Gamma)\square\Big]_\Gamma\,, \end{aligned} \tag{23a}$$

$$\begin{aligned}\mathrm{D}_{q_k}\phi(q)[\square] =& \left[\big(\partial_{q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}}) - \operatorname{div}\partial_{\nabla q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}}, \nabla q_{\mathrm{B}})\big)\square\right]_{\Omega\setminus\Gamma} \\ &+ \sum_{i\in\{+,-\}} \Big[\big(\partial_{q_{k_i}}\phi_\Gamma(q_+, q_-, q_\Gamma) + \partial_{\nabla q_k}\phi_{\mathrm{B}}(q_i, \nabla q_i)\cdot \mathrm{n}_i\big)\square\Big]_\Gamma\,, \end{aligned} \tag{23b}$$

$$\alpha * \mathrm{D}_{q_k}\phi(q)[\square] = \big[\big(\alpha\partial_{q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}},\nabla q_{\mathrm{B}}) - \operatorname{div}\big(\alpha\partial_{\nabla q_k}\phi_{\mathrm{B}}(q_{\mathrm{B}},\nabla q_{\mathrm{B}})\big)\big)\square\big]_{\Omega\setminus\Gamma} + \sum_{i\in\{+,-\}}\Big[\big(\alpha\partial_{q_{k_i}}\phi_{\Gamma}(q_+,q_-,q_{\Gamma}) + \alpha\partial_{\nabla q_k}\phi_{\mathrm{B}}(q_i,\nabla q_i)\cdot \mathrm{n}_i\big)\square\Big]_{\Gamma}\,. \tag{23c}$$

In general there is the following equivalence in a weak sense

$$\alpha * \mathrm{D}_{q_k}\phi(q)[\tilde{q}_k] = \alpha\delta_{q_k}\phi(q)[\tilde{q}_k]\,. \tag{24}$$

**Dual dissipation potentials.** In the same manner, the notation introduced in (20)–(23) is also applied for dual dissipation potentials $\Psi^* = \Psi^*_{\mathrm{B}} + \Psi^*_{\Gamma} : \mathcal{Q}\times\mathcal{Q}^* \to [0,\infty]$ and the dual states $\xi := (\xi_{\mathrm{B}}, \xi_{\Gamma}) \in \mathcal{Q}^*$ with $\xi_{\mathrm{B}} \in \mathcal{Q}^*_{\mathrm{B}}$ and $\xi_{\Gamma} \in \mathcal{Q}^*_{\Gamma}$. In particular, we will see that the corresponding Onsager operator is thus given by

$$\mathbb{K}(q;\xi) := \mathrm{D}_{\xi_{\mathrm{B}}}\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\xi_{\mathrm{B}}) + \mathrm{D}_{\xi}\Psi^*_{\Gamma}(q;\xi)\,. \tag{25}$$

**Geometric structures.** Also state-dependent geometric structures $\mathbb{J} = \mathbb{J}_{\mathrm{B}} + \mathbb{J}_{\Gamma} : \mathcal{Q}\times\mathcal{Q}^* \to \mathcal{Q}$, and $\mathbb{K} = \mathbb{K}_{\mathrm{B}} + \mathbb{K}_{\Gamma} : \mathcal{Q}\times\mathcal{Q}^* \to \mathcal{Q}$ are composed of bulk and interfacial contributions with $\mathcal{Q} = \mathcal{Q}_{\mathrm{B}}\times\mathcal{Q}_{\Gamma}$.

## 3.2 Direct implications for geometric structures

Next, we discuss the defining properties of the geometric structures with bulk-interface interaction in more detail. In particular, we have:

**Lemma 3.3** (Properties of dual dissipation potentials)**.** *Let the setup of Def. 3.1 and Section 3.1 be satisfied. Consider a dual dissipation potential $\Psi^* = \Psi^*_{\mathrm{B}} + \Psi^*_{\Gamma} : \mathcal{Q}\times\mathcal{Q}^* \to [0,\infty]$ of the form*

$$\Psi^*(q;\xi) = \int_{\Omega\setminus\Gamma} \psi^*_{\mathrm{B}}(q_{\mathrm{B}};\xi_{\mathrm{B}},\nabla\xi_{\mathrm{B}})\,\mathrm{d}x + \int_{\Gamma}\psi^*_{\Gamma}(q_{\Gamma\gamma};\xi_{\Gamma\gamma})\mathrm{d}\mathcal{H}^{d-1}\,. \tag{26}$$

1 *Assume that $\Psi^*(q;\cdot) : \mathcal{Q}^* \to [0,\infty]$ is convex for all $q \in \mathcal{Q}$. Hence, both $\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot) : \mathcal{Q}^*_{\mathrm{B}} \to [0,\infty]$ and $\Psi^*_{\Gamma}(q;\cdot) : \mathcal{Q}^* \to [0,\infty]$ are convex for all $q = (q_{\mathrm{B}}, q_{\Gamma}) \in \mathcal{Q}$.*

2 *Assume that $\Psi^*(q;\cdot) : \mathcal{Q}^* \to [0,\infty]$ is convex for all $q \in \mathcal{Q}$ and in addition also that $\Psi^*(q;0) = 0$ for all $q \in \mathcal{Q}$. Then there holds*

$$\langle \xi, \tilde{q}\rangle_{\mathcal{Q}} \geq 0 \text{ for all } (q,\xi) \in \mathcal{Q}\times\mathcal{Q}^* \text{ and for all } \tilde{q} \in \partial_{\xi}\Psi^*(q;\xi)\,. \tag{27a}$$

*Moreover, also $\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot)$ and $\Psi^*_{\Gamma}(q;\cdot)$ satisfy*

$$\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};0) = 0 \text{ for all } q_{\mathrm{B}} \in \mathcal{Q}_{\mathrm{B}}\,, \qquad \Psi^*_{\Gamma}(q;0) = 0 \text{ for all } q \in \mathcal{Q} \tag{27b}$$

$$\langle \xi_{\mathrm{B}}, \tilde{q}_{\mathrm{B}}\rangle_{\mathcal{Q}_{\mathrm{B}}} \geq 0 \text{ for all } \xi_{\mathrm{B}} \in \mathcal{Q}^*_{\mathrm{B}},\ \tilde{q}_{\mathrm{B}} \in \partial_{\xi_{\mathrm{B}}}\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\xi_{\mathrm{B}})\,, \tag{27c}$$

$$\langle \xi, \tilde{q}\rangle_{\mathcal{Q}} \geq 0 \text{ for all } \xi \in \mathcal{Q}^*,\ \tilde{q} \in \partial_{\xi}\Psi^*_{\Gamma}(q;\xi)\,. \tag{27d}$$

*Furthermore, if $\Psi^*(q;\cdot)$ is Gâteaux-differentiable for all $q \in \mathcal{Q}$, then also $\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot)$ and $\Psi^*_{\Gamma}(q;\cdot)$ are so, and vice versa.*

3 *In addition to the prerequisites of 2. assume that for all $q \in \mathcal{Q}$ the potential $\Psi^*(q;\cdot) : \mathcal{Q}^* \to [0,\infty]$ is quadratic and Gâteaux-differentiable. Then $\mathbb{K}(q) = \mathrm{D}_{\xi}\Psi^*(q;\cdot) : \mathcal{Q}^* \to \mathcal{Q}$ is a linear, symmetric and positively semidefinite operator, and so are its bulk part $\mathbb{K}_{\mathrm{B}}(q_{\mathrm{B}}) = \mathrm{D}_{\xi_{\mathrm{B}}}\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot)$ and its boundary part $\mathbb{K}_{\Gamma}(q) = \mathrm{D}_{\xi}\Psi^*_{\Gamma}(q;\cdot)$.*

*Proof.* **To 1.:** Convexity of $\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot)$ and $\Psi^*_{\Gamma}(q;\cdot)$ is equivalent to the convexity of the densities $\psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot,\cdot)$, $\psi^*_{\Gamma}(q_{\Gamma\gamma};\cdot)$. Since these two densities have different supports, the assertion follows.

**To 2.:** By the definition of the subdifferential for convex potentials (12) we deduce that $\Psi^*(q;0) - \Psi^*(q;\xi) \geq \langle \tilde{q}, -\xi\rangle_{\mathcal{Q}}$ for all $\xi \in \mathcal{Q}^*$, $\tilde{q} \in \partial_\xi \Psi^*(q;\xi)$. Using that $\Psi^*(q;0) = 0$ and rearranging terms results in (27a). Moreover, since the densities $\psi^*_{\mathrm{B}}$ and $\psi^*_{\Gamma}$ have different supports, the first statement of (27c) and (27d) follows. Furthermore, by 1., both potentials $\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot)$ and $\Psi^*_{\Gamma}(q;\cdot)$ are convex. Thus the second statement of (27c) and (27d) is obtained by repeating the argument for (27a). Again, since the densities $\psi^*_{\mathrm{B}}$ and $\psi^*_{\Gamma}$ have different supports, the Gâteaux-differentiability of $\Psi^*(q;\cdot)$ is equivalent to the Gâteaux-differentiability of $\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot)$ and $\Psi^*_{\Gamma}(q;\cdot)$.

**To 3.:** The potential $\Psi^*(q;\cdot)$ is quadratic and Gâteaux-differentiable if and only if $\Psi^*_{\mathrm{B}}(q_{\mathrm{B}};\cdot)$ and $\Psi^*_{\Gamma}(q;\cdot)$ are so. Hence their derivatives are linear, symmetric operators. Positive semidefiniteness follows from (27c), resp. (27d). □

At this point we also address canonical Poisson structures for bulk-interface interaction with an immediate statement. With the aid of transformation maps, this finding will be transferred to the non-canonical case in Sec. 3.4, see Lemma 3.8.

**Lemma 3.4** (Properties of canonical Poisson structures)**.** *Let the setup of Def. 3.1 and Section 3.7 be satisfied.Further let $\mathbb{J}_{\mathrm{B}} : \mathcal{Q}^*_{\mathrm{B}} \to \mathcal{Q}_{\mathrm{B}}$ and $\mathbb{J}_{\Gamma} : \mathcal{Q}^*_{\mathrm{B}} \times \mathcal{Q}^*_{\Gamma} \to \mathcal{Q}_{\mathrm{B}} \times \mathcal{Q}_{\Gamma}$ be both in canonical form. Hence $\mathbb{J}_{\mathrm{B}}$ and $\mathbb{J}_{\Gamma}$ are antisymmetric, satisfy the Leibniz rule as well as Jacobi's identity. Moreover, also $\mathbb{J} = \mathbb{J}_{\mathrm{B}} + \mathbb{J}_{\Gamma}$ is in canonical form, thus antisymmetric and satisfies the Leibniz rule as well as Jacobi's identity.*

In addition, also the NIC 14 can be shown to hold true for geometric structures and functionals with bulk-interface interaction of the type introduced in Sec. 3.1. This also results in the validity of energy conservation and entropy production and is consistent with the fact that the coupled bulk-interface system is assumed to be thermodynamically closed, cf. Def. 3.1.

**Lemma 3.5** (NIC for GENERIC bulk-interface systems)**.** *Under the prerequisites of Lemma 3.3 consider energy and entropy functionals of the form* (20)*. Further assume that $\Psi^*$ and $\mathcal{E}$ satisfy the generalized NIC* (15)*. Then*

$$\langle \mathrm{D}\mathcal{E}(q), \tilde{q}\rangle_{\mathcal{Q}} = 0 \text{ for all } q \in \mathcal{Q}, \xi \in \mathcal{Q}^*, \text{ and all } \tilde{q} \in \partial_\xi \Psi^*(q;\xi)\,, \tag{28}$$

*and thus, for solutions $q \in L^2(0,T;\mathcal{Q}) \cap H^1(0,T;\mathcal{Q}^*)$ of* (13) *the energy conservation and entropy production hold true, i.e.,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(q(t)) = 0 \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(q(t)) \geq 0 \quad \text{for all } t \in [0,\mathrm{T}]. \tag{29}$$

*Moreover the generalized NIC* (15) *as well as properties* (29) *hold true even separately for the bulk and boundary contributions of $\mathcal{E} = \mathcal{E}_{\mathrm{B}} + \mathcal{E}_{\Gamma}$, $\mathcal{S} = \mathcal{S}_{\mathrm{B}} + \mathcal{S}_{\Gamma}$, and $\Psi^* = \Psi^*_{\mathrm{B}} + \Psi^*_{\Gamma}$.*

*Proof.* By the generalized NIC (15) we have for all $q \in \mathcal{Q}$, for all $\xi \in \mathcal{Q}^*$, for all $\tilde{q} \in \partial_\xi \Psi^*(q;\xi)$, and for all $\lambda \in \mathbb{R}$

$$0 = \Psi^*(q;\xi + \lambda \mathrm{D}\mathcal{E}(q)) - \Psi^*(q;\xi) \geq \langle \lambda \mathrm{D}\mathcal{E}(q), \tilde{q}\rangle_{\mathcal{Q}}\,.$$

Choosing $\lambda = 1$ and $\lambda = -1$ gives (28). Now energy conservation follows by direct calculation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(q(t)) = \langle \mathrm{D}\mathcal{E}(q), \dot{q}\rangle_{\mathcal{Q}} = \langle \mathrm{D}\mathcal{E}(q), \mathbb{J}\mathrm{D}\mathcal{E}(q) + \tilde{q}\rangle_{\mathcal{Q}} = 0 + 0 = 0$$

using the chain rule, the antisymmetry of $\mathbb{J}$, cf. (3), and (28). With similar arguments also the entropy production of the system is verified:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(q(t)) = \langle \mathrm{D}\mathcal{S}(q), \dot{q}\rangle_{\mathcal{Q}} = \langle \mathrm{D}\mathcal{S}(q), \mathbb{J}\mathrm{D}\mathcal{E}(q) + \tilde{q}\rangle_{\mathcal{Q}} \geq 0 + 0\,,$$

where the first $0$ arises by the antisymmetry of $\mathbb{J}$ together with the NIC $\mathbb{J}\mathrm{D}\mathcal{S}(q) = 0$ and the inequality is due to (27a). This finishes the proof of (29).

Since the densities $\psi_{\mathrm{B}}^*$ and $\psi_{\Gamma}^*$ as well as $E_{\mathrm{B}}$ and $E_{\Gamma}$ have different supports, the generalized NIC (15) has to be satisfied separately for $\Psi^*(q_{\mathrm{B}}; \mathrm{D}_{\mathrm{B}}\mathcal{E}_{\mathrm{B}}(q_{\mathrm{B}})$ and $\Psi_{\Gamma}^*(q; \mathrm{D}_q\mathcal{E}_{\Gamma}(q))$ in order to hold true for $\Psi^*$ and $\mathcal{E}$. Accordingly also the relations $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\mathrm{B}}(q_{\mathrm{B}}(t)) = 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\Gamma}(q(t)) = 0$ as well as $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}_{\mathrm{B}}(q_{\mathrm{B}}(t)) \geq 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}_{\Gamma}(q(t)) \geq 0$ are obtained separately for the bulk and boundary contributions. □

**Remark 3.6** (Comparison with [Ött06])**.** Lemmata 3.3 and 3.4 show that with the setup of Def. 3.1 and Sec. 3.1 the characteristic properties of GENERIC systems $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ are satisfied separately by the bulk system $(\mathcal{Q}_{\mathrm{B}}, \mathcal{E}_{\mathrm{B}}, \mathcal{S}_{\mathrm{B}}, \mathbb{J}_{\mathrm{B}}, \mathbb{K}_{\mathrm{B}})$ and by the surface system $(\mathcal{Q}, \mathcal{E}_{\Gamma}, \mathcal{S}_{\Gamma}, \mathbb{J}_{\Gamma}, \mathbb{K}_{\Gamma})$. This finding essentially rests on our definition of the derivatives and operations (21)–(24) for functionals with bulk and boundary contributions, i.e. considering the derivatives as distributions rather than classical functions. When starting from the abstract definition of variations and functional derivatives (21a)–(21c) of functionals defined on Banach spaces, relations (21d)–(24) arise as a natural consequence. We refer to [Ött06], where the boundary terms arising from the bulk contributions by integration by parts, are attributed to the boundary part of the system. Consequently, neither the bulk nor the boundary system satisfies the characteristic properties of a GENERIC system, but the sum of the two does. We stress that our approach and [Ött06] lead to the same bulk-interface systems. ⋆

## 3.3 Weak form of GENERIC as a formalism for bulk-interface systems

Based on the definitions given in Def. 3.1 and Sec. 3.1 we now introduce a GENERIC formalism for systems with bulk-interface interaction and open systems in terms of a weak formulation. In this way, the bulk equations have to hold in a weak sense and the coupling conditions along $\Gamma$ naturally appear also in a weak sense. *Let $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ be a system with bulk and surface contributions as described in Def. 3.1 and Sec. 3.1, with the mapping properties $\mathcal{E} = \mathcal{E}_{\mathrm{B}} + \mathcal{E}_{\Gamma} : \mathcal{Q} \to \mathbb{R}$, $\mathcal{S} = \mathcal{S}_{\mathrm{B}} + \mathcal{S}_{\Gamma} : \mathcal{Q} \to \mathbb{R}$, $\mathbb{J} = \mathbb{J}_{\mathrm{B}} + \mathbb{J}_{\Gamma} : \mathcal{Q}^* \to \mathcal{Q}$, and $\mathbb{K} = \mathbb{K}_{\mathrm{B}} + \mathbb{K}_{\Gamma} : \mathcal{Q}^* \to \mathcal{Q}$ with $\mathcal{Q} = \mathcal{Q}_{\mathrm{B}} \times \mathcal{Q}_{\Gamma}$. A weak formulation for $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ is given by:*

$$\begin{aligned}\langle \tilde{\xi}, \dot{q}\rangle_{\mathcal{Q}} &= \langle \tilde{\xi}_{\mathrm{B}}, \dot{q}_{\mathrm{B}}\rangle_{\mathcal{Q}_{\mathrm{B}}} + \langle \tilde{\xi}_{\Gamma}, \dot{q}_{\Gamma}\rangle_{\mathcal{Q}_{\Gamma}} = \langle \tilde{\xi}, \mathbb{J}\mathrm{D}\mathcal{E}(q) + \mathbb{K}\mathrm{D}\mathcal{S}(q)\rangle_{\mathcal{Q}} \\ &= \langle \tilde{\xi}_{\mathrm{B}}, \mathbb{J}_{\mathrm{B}}(q_{\mathrm{B}})\mathrm{D}_{q_{\mathrm{B}}}\mathcal{E}_{\mathrm{B}}(q_{\mathrm{B}}) + \mathbb{K}_{\mathrm{B}}(q_{\mathrm{B}})\mathrm{D}_{q_{\mathrm{B}}}\mathcal{S}_{\mathrm{B}}(q_{\mathrm{B}})\rangle_{\mathcal{Q}_{\mathrm{B}}} \\ &\quad + \langle \tilde{\xi}_{\Gamma\gamma}, \mathbb{J}_{\Gamma}(q_{\Gamma\gamma})\mathrm{D}_{q_{\Gamma\gamma}}\mathcal{E}_{\Gamma}(q_{\Gamma\gamma}) + \mathbb{K}_{\Gamma}(q_{\Gamma\gamma})\mathrm{D}_{q_{\Gamma\gamma}}\mathcal{S}_{\Gamma}(q_{\Gamma\gamma})\rangle_{\mathcal{Q}_{\Gamma\gamma}}\end{aligned} \tag{30}$$

*for all $\tilde{\xi} = (\tilde{\xi}_{\mathrm{B}}, \tilde{\xi}_{\Gamma}) \in \tilde{\mathcal{Q}} \subset \mathcal{Q}^*$ for with $\tilde{\mathcal{Q}} = \tilde{\mathcal{Q}}_{\mathrm{B}} \times \tilde{\mathcal{Q}}_{\Gamma}$ a suitable space of test functions. Here, $q_{\Gamma\gamma}$ is defined as in* (19) *and $\tilde{\xi}_{\Gamma\gamma} = (\tilde{\xi}_{+\gamma}, \tilde{\xi}_{-\gamma}, \tilde{\xi}_{\Gamma}) \in (\gamma\mathcal{Q})^* \times \mathcal{Q}_{\Gamma}^*$.* At the example of heat conduction we now illustrate how the weak form of GENERIC arises from the definition of functional derivatives for functionals with bulk-interface interaction and how the interfacial coupling naturally emerge from this weak form.

**Example 3.7** (Heat transfer for bulk-interface and open systems)**.** In the following we discuss the Onsager structure for heat conduction taking into account different interfacial Osager operators along $\Gamma$ thus resulting in different coupling conditions.

*Heat conduction in the bulk* $\Omega\backslash\Gamma = \Omega_+ \cup \Omega_-$*:* The dual dissipation potential in the bulk is defined as

$$\Psi^*_{\mathrm{B}}(\theta;\cdot) : \mathcal{Q}^* \to \mathbb{R},\ \Psi^*_{\mathrm{B}}(\theta;\xi) := \sum_{i\in\{+,-\}} \int_{\Omega_i} \tfrac{\theta^2\kappa(\theta)}{2} \big|\nabla\big(\tfrac{\xi}{\mathrm{D}_\theta E}\big)\big|^2 \,\mathrm{d}x\,. \tag{31}$$

Hence, the first variation in $\xi$ reads

$$\delta_\xi \Psi^*_{\mathrm{B}}(\theta;\xi)[\tilde\xi] := \sum_{i\in\{+,-\}} \int_{\Omega_i} \theta^2\kappa(\theta) \nabla\big(\tfrac{\xi}{\mathrm{D}_\theta E}\big) \cdot \nabla\big(\tfrac{\tilde\xi}{\mathrm{D}_\theta E}\big)\,\mathrm{d}x\,. \tag{32}$$

We formally distinguish it from the functional derivative $\mathrm{D}_\xi \Psi^*_{\mathrm{B}}(\theta;\xi)$, which is obtained from $\delta_\xi\Psi^*_{\mathrm{B}}$ by an integration by parts, i.e.,

$$\begin{aligned}
\mathrm{D}_\xi \Psi^*_{\mathrm{B}}(\theta;\xi)[\tilde\xi] = &\sum_{i\in\{+,-\}} \int_{\Omega_i} -\operatorname{div} \theta^2\kappa(\theta)\nabla\big(\tfrac{\xi}{\mathrm{D}_\theta E}\big)\tfrac{\tilde\xi}{\mathrm{D}_\theta E}\,\mathrm{d}x \\
&+ \sum_{i\in\{+,-\}} \int_{\Gamma_i} \gamma_i\Big(\theta_i^2\kappa(\theta_i)\nabla\big(\tfrac{\xi_i}{\mathrm{D}_\theta E_i}\big)\Big)\cdot \mathrm{n}_i\,\gamma_i\big(\tfrac{\tilde\xi_i}{\mathrm{D}_\theta E_i}\big)\,\mathrm{d}\mathcal{H}^{d-1} \\
=:&\langle \mathbb{K}_{\mathrm{B}}(\theta)\,\xi, \tilde\xi\rangle_{\mathcal{Q}}\,,
\end{aligned}$$

and we introduce the Onsager operator

$$\mathbb{K}_{\mathrm{B}}(\theta) = \sum_{i\in\{+,-\}} \Big[\tfrac{-1}{\mathrm{D}_\theta E}\operatorname{div}\Big(\theta^2\kappa(\theta)\nabla\big(\tfrac{\square}{\mathrm{D}_\theta E}\big)\Big)\Big]_{\Omega_i} + \Big[\gamma_i\Big(\tfrac{\theta_i^2\kappa_i(\theta_i)}{\mathrm{D}_\theta E_i}\nabla\big(\tfrac{\square}{\mathrm{D}_\theta E}\big)\Big)\cdot \mathrm{n}_i\Big]_{\Gamma_i}\,. \tag{33}$$

*Ideal heat transfer across the perfectly conducting interface* $\Gamma$*:* At the perfectly conducting interface $\Gamma$ all quantities are continuous, which implies

$$\gamma_+\tilde\xi_+ = \gamma_-\tilde\xi_- \ \text{ for all } \tilde\xi \in \mathcal{Q}^*, \tag{34a}$$

$$\gamma_+\Big(\tfrac{\theta_+^2\kappa_+(\theta_+)}{\mathrm{D}_\theta E_+}\nabla\big(\tfrac{\xi_+}{\mathrm{D}_\theta E_+}\big)\Big)\cdot \mathrm{n}_+ = -\gamma_-\Big(\tfrac{\theta_-^2\kappa_-(\theta_-)}{\mathrm{D}_\theta E_-}\nabla\big(\tfrac{\xi_-}{\mathrm{D}_\theta E_-}\big)\Big)\cdot \mathrm{n}_-\,. \tag{34b}$$

Furthermore, $\mathbb{K}_{\mathrm{B}}$ satisfies properties (8) as well as NIC (14).

*Heat transfer across the imperfect interface* $\Gamma$*:* We assume that the heat transfer through $\Gamma$ is regulated by the heat transfer coefficient $\hat\kappa_\Gamma(\gamma_+\theta_+, \gamma_-\theta_-)$. In this spirit we introduce the quadratic dual dissipation potential along $\Gamma$, for every $\xi_\gamma \in \operatorname{dom}(\Psi_\Gamma(\theta_\gamma;\cdot))$

$$\Psi^*_\Gamma(\theta_\gamma;\xi_\gamma) := \int_\Gamma \tfrac{\hat\kappa_\Gamma(\gamma_+\theta_+,\gamma_-\theta_-)}{2}\Big|\gamma_+\big(\tfrac{\xi_+}{\mathrm{D}_\theta E_+}\big) - \gamma_-\big(\tfrac{\xi_-}{\mathrm{D}_\theta E_-}\big)\Big|^2\,\mathrm{d}\mathcal{H}^{d-1} \tag{35}$$

and we find for all $\xi_\gamma, \tilde\xi_\gamma \in \operatorname{dom}(\Psi_\Gamma(\theta_\gamma;\cdot))$ that

$$\begin{aligned}
\mathrm{D}_{\xi_\gamma}\Psi^*_\Gamma(\theta_\gamma;\xi_\gamma)\big[\tilde\xi_\gamma\big] &= \int_\Gamma \hat\kappa_\Gamma(\theta_+,\theta_-)\Big(\big(\tfrac{\xi_+}{\mathrm{D}_\theta E_+}\big) - \big(\tfrac{\xi_-}{\mathrm{D}_\theta E_-}\big)\Big)\Big(\big(\tfrac{\tilde\xi_+}{\mathrm{D}_\theta E_+}\big) - \big(\tfrac{\tilde\xi_-}{\mathrm{D}_\theta E_-}\big)\Big)\,\mathrm{d}\mathcal{H}^{d-1} \\
&= \big\langle \mathbb{K}_\Gamma(\theta_\gamma)\xi_\gamma, \tilde\xi_\gamma\big\rangle_{\operatorname{dom}(\Psi_\Gamma(\theta_\gamma;\cdot))}\,.
\end{aligned} \tag{36}$$

Clearly, $\mathbb{K}_\Gamma(\theta_\gamma)$ is symmetric and positively semidefinite provided that $\hat\kappa_\Gamma(\theta_\Gamma) \geq 0$. Also NIC (14) holds true since for all $\tilde\xi_\gamma = (\tilde\xi_+, \tilde\xi_-)^\top$ we have

$$\begin{aligned}
&\big\langle \mathbb{K}_\Gamma(\theta_\gamma)(\mathrm{D}_\theta E)_\Gamma, \tilde\xi_\gamma\big\rangle_{\operatorname{dom}(\Psi_\Gamma(\theta_\gamma;\cdot))} \\
&\quad= \int_\Gamma \hat\kappa_\Gamma(\theta_+,\theta_-)\Big(\tfrac{\mathrm{D}_\theta E_+}{\mathrm{D}_\theta E_+} - \tfrac{\mathrm{D}_\theta E_-}{\mathrm{D}_\theta E_-}\Big)\Big(\tfrac{\tilde\xi_+}{\mathrm{D}_\theta E_+} - \tfrac{\tilde\xi_-}{\mathrm{D}_\theta E_-}\Big)\,\mathrm{d}\mathcal{H}^{d-1} = 0\,.
\end{aligned} \tag{37}$$

Thus, in view of (33) and (37), the Onsager operator of the full coupled system is

$$\mathbb{K}(\theta) = \mathbb{K}_{\mathrm{B}}(\theta) + \mathbb{K}_{\Gamma}(\theta_\gamma) \tag{38}$$

and $\mathbb{K}(\theta)$ is symmetric, positively semidefinite, and satisfies the NIC (14).

Now the evolution equation (7) can be understood in a weak form such that for a.a. $t \in (0, \mathsf{T})$ and for all $\tilde{\xi} \in \tilde{\mathcal{Q}} = H^1(\Omega\backslash\Gamma)$ there holds

$$\begin{aligned}\langle \dot\theta, \tilde\xi\rangle_{\tilde{\mathcal{Q}}} &= \langle \mathbb{K}(\theta)\mathrm{D}_\theta\mathcal{S}(\theta), \tilde\xi\rangle_{\tilde{\mathcal{Q}}} \\ &= \langle \mathbb{K}_{\mathrm{B}}(\theta)\mathrm{D}_\theta\mathcal{S}(\theta), \tilde\xi\rangle_{H^1(\Omega\backslash\Gamma)} + \langle \mathbb{K}_\Gamma(\theta_\Gamma)\mathrm{D}_\theta\mathcal{S}_\Gamma(\theta), \tilde\xi_\Gamma\rangle_{H^{1/2}(\Gamma)}\,.\end{aligned} \tag{39}$$

For a closed system, the heat flux through the boundary is $0$ pointwise, i.e.

$$\theta^2\kappa(\theta)\nabla\big(\tfrac{\xi}{\mathrm{D}_\theta E}\big)\tfrac{1}{\mathrm{D}_\theta E}\cdot\nu_{\partial\Omega} = 0 \qquad \text{on} \quad \partial\Omega\,.$$

Hence, choosing test functions $\tilde\xi = \mathrm{D}_\theta E\,\hat\xi$ with $\hat\xi \in \tilde{\mathcal{Q}}$ and using the Gibbs relation, for a.a. $t \in (0, \mathsf{T})$, it holds in a weak sense in $\mathcal{Q} = \tilde{\mathcal{Q}}^*$ it holds

$$\mathrm{D}_\theta E\,\dot\theta = -\operatorname{div}\big(\theta^2\kappa(\theta)\nabla\tfrac{1}{\theta}\big)\,, \quad \text{in } \Omega\backslash\Gamma\,, \tag{40a}$$

together with the following transmission conditions along $\Gamma$

$$\gamma_+\Big(\tfrac{\theta_+^2\kappa_+(\theta_+)}{\mathrm{D}_\theta E_+}\nabla\big(\tfrac{1}{\theta_+}\big)\Big)\cdot \mathrm{n}_+ \;=\; -\gamma_-\Big(\tfrac{\theta_-^2\kappa_-(\theta_-)}{\mathrm{D}_\theta E_-}\nabla\big(\tfrac{1}{\theta_-}\big)\Big)\cdot \mathrm{n}_-\,, \tag{40b}$$

$$\gamma_+\Big(\tfrac{\theta_+^2\kappa_+(\theta_+)}{\mathrm{D}_\theta E_+}\nabla\big(\tfrac{1}{\theta_+}\big)\Big)\cdot \mathrm{n}_+ \;=\; -\hat\kappa_\Gamma(\theta_\gamma)\big(\tfrac{1}{\theta_+}-\tfrac{1}{\theta_-}\big) = \tfrac{\hat\kappa_\Gamma(\theta_\gamma)}{\theta_+\theta_-}\big[\!\big[\theta\big]\!\big]\,, \tag{40c}$$

complemented by homogeneous boundary conditions along $\partial\Omega$ and by an initial condition.We point out that the transmission conditions (40b) & (40c) are also obtained e.g. in [GB13, RCC$^+$16] for interfaces in local equilibrium.

*Ideal heat transfer across the external boundary $\partial\Omega_+ = \Gamma$:* In the setting of scenario 2 from Def. 3.1, above considerations help to formulate proper boundary conditions for non-closed systems. In this case, $\Omega_+$ is a bounded domain which is connected to a reservoir $\Omega_-$. Evolution equation (40) then has to be satisfied only in $\Omega_+$ whereas the part of the system on $\Omega_-$ is not of interest. For a perfectly conducting boundary $\Gamma$ and for a given function $h$ we thus set

$$-\gamma_-\Big(\tfrac{\theta_-^2\kappa_-(\theta_-)}{\mathrm{D}_\theta E_-}\nabla\big(\tfrac{\xi_-}{\mathrm{D}_\theta E_-}\big)\Big)\cdot \mathrm{n}_- := h. \tag{41}$$

In other words, the inhomogeneous Neumann boundary condition $h$ is implemented in the above deduced GENERIC system by appropriately adjusting the functions $\kappa_-$ on $\Omega_-$, $E_-(\theta_-)$ and by making an appropriate choice for $\xi_-$.

In case of an imperfectly conducting boundary we are free to choose $\theta_-$ and the coefficient functions $\kappa_-(\theta_-)$, $E_-(\theta_-)$, and $\hat\kappa_\Gamma(\theta_\Gamma)$ for a given function $h$ such that

$$-\tfrac{\theta_-^2\kappa_-(\theta_-)}{\mathrm{D}_\theta E_-}\nabla\big(\tfrac{1}{\theta_-}\big)\cdot \mathrm{n}_- = h \quad \text{and} \quad \tfrac{\hat\kappa_\Gamma(\theta_\Gamma)}{\theta_+\theta_-}\big[\!\big[\theta\big]\!\big] = h\,. \tag{42}$$

Again, the inhomogeneous Neumann boundary condition is implemented in the above GENERIC system by appropriately adjusting the coefficient functions on $\Omega_-$ and $\Gamma$ and by making an appropriate choice for $\xi_-$.

In both cases (perfect or imperfect), this neither interferes with the symmetry of $\mathbb{K}$ nor with the validity of NIC (14), but to ensure positive semidefiniteness of $\mathbb{K}$ may require to restrict the choices of $h$. $\star$

We refer to Section 4 to see (30) in application for specific examples of bulk-interface systems related to delamination processes.

### 3.4 Tools for dissipative solids with bulk-interface interaction

In [Mie11a, Sec. 2.4] and [ZPT21, Sec. 3.4] it was established that the GENERIC structure of thermodynamically closed systems is preserved under similarity transformations. In particular, this approach can be used to facilitate the verification of the structural properties of the system, such as the NIC (14). For this, first consider a thermodynamically closed system described by the states $q_\tau = (w, \tau) \in \mathcal{Q}_\tau$, where $\tau \in \{E, U, S, \theta\}$ represents the thermodynamic variable and $w \in \mathbb{R}^N$ collects the remaining state variables. For an integral functional $\mathcal{H} : \mathcal{Q}_\tau \to \mathbb{R}$ with density $H$ (and $H$ as a placeholder for $E, U, S$) we introduce the map

$$\mathrm{T}_{\tau\to H} : \mathcal{Q}_\tau \to \mathcal{Q}_H,\ q_\tau := (w, \tau) \mapsto q_H := (w, H) \tag{43}$$

and its inverse $\mathrm{T}_{H\to\tau} = \mathrm{T}^{-1}_{\tau\to H}$. Calculation of the Fréchet derivative of $\mathrm{T}_{H\to\tau}$ thus gives

$$\mathbb{L}_H := \mathrm{DT}_{H\to\tau}(q_H) = \mathrm{DT}_{\tau\to H}(q_\tau)^{-1} = \begin{pmatrix} I & 0 \\ \delta_w H(q_\tau) & \partial_\tau H(q_\tau) \end{pmatrix}^{-1} \tag{44}$$

and leads to the relations

$$\mathbb{L}_H = \begin{pmatrix} I & 0 \\ -\frac{1}{\partial_\tau H}\delta_w H & \frac{1}{\partial_\tau H} \end{pmatrix} \quad \text{and} \quad \mathbb{L}_H^* = \begin{pmatrix} I & -\frac{\square}{\partial_\tau H} * \mathrm{D}_w H \\ 0 & \frac{1}{\partial_\tau H} \end{pmatrix}.$$

More generally, for some linear operator $\mathbb{A}_H : \mathcal{Q}_w^* \to \mathcal{Q}_w^*$ with adjoint $\mathbb{A}_H^*$ we set

$$\mathbb{L}_H = \begin{pmatrix} \mathbb{A}_H & 0 \\ -\frac{\delta_w H \circ \mathbb{A}_H}{\partial_\tau H} & \frac{1}{\partial_\tau H} \end{pmatrix} \quad \text{and} \quad \mathbb{L}_H^* = \begin{pmatrix} \mathbb{A}_H^* & \mathbb{A}_H^* \circ (-\frac{\square}{\partial_\tau H} * \mathrm{D}_w H) \\ 0 & \frac{1}{\partial_\tau H} \end{pmatrix}. \tag{45}$$

In this way there clearly holds

$$\mathbb{L}_H^* \mathrm{D}\mathcal{H} \equiv \mathbb{L}_H^* \mathrm{D}H = (0, 1)^\top \tag{46}$$

and the NIC (14) is ensured by assuming that the Poisson and the Onsager operator of a GENERIC system in the variables $q_\tau$ can be composed as

$$\mathbb{J}(q_\tau) := \mathbb{L}_S \mathbb{J}^0 \mathbb{L}_S^* \quad \text{and} \quad \mathbb{K}(q_\tau) := \mathbb{L}_E \mathbb{K}^0 \mathbb{L}_E^* \quad \text{with} \quad \mathbb{J}^0 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 = \mathbb{K}^0 \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{47}$$

Here, $\mathbb{J}^0 : \mathcal{Q}_S^* \to \mathcal{Q}_S$ is a Poisson structure and $\mathbb{K}^0 : \mathcal{Q}_E^* \to \mathcal{Q}_E$ is an Onsager operator on the state spaces $\mathcal{Q}_S, \mathcal{Q}_E$ with homogeneous boundary conditions.

We observe now that similar relations can also be established for systems with bulk-interface interaction: Following the notation of Sec. 3.1 we assume that the bulk energy and entropy densities are given through $E_{\mathrm{B}}(w_{\mathrm{B}}, \nabla w_{\mathrm{B}}, \tau_{\mathrm{B}}) = E_+(w_+, \nabla w_+, \tau_+) + E_-(w_-, \nabla w_-, \tau_-)$ and $S_{\mathrm{B}}(w_{\mathrm{B}}, \nabla w_{\mathrm{B}}, \tau_{\mathrm{B}}) = S_+(w_+, \nabla w_+, \tau_+) + S_-(w_-, \nabla w_-, \tau_-)$. For simplicity, we assume that all variables, particularly $\tau_\pm$, have well defined traces on $\Gamma$. Since $\Omega_+$ and $\Omega_-$ are disjoint, we can follow (47) and find the bulk operators

$$\mathbb{J}_{\mathrm{B}}(q_{\tau_{\mathrm{B}}}) := \mathbb{L}_{S_+} \mathbb{J}_+^0 \mathbb{L}_{S_+}^* + \mathbb{L}_{S_-} \mathbb{J}_-^0 \mathbb{L}_{S_-}^* \quad \text{with} \quad \mathbb{J}_\pm^0 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 \quad \text{and} \tag{48a}$$

$$\mathbb{K}_{\mathrm{B}}(q_{\tau_{\mathrm{B}}}) := \mathbb{L}_{E_+} \mathbb{K}_+^0 \mathbb{L}_{E_+}^* + \mathbb{L}_{E_-} \mathbb{K}_-^0 \mathbb{L}_{E_-}^* \quad \text{with} \quad \mathbb{K}_\pm^0 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0\,. \tag{48b}$$

Now $\mathbb{J}_\pm^0 : \mathcal{Q}_{S_\pm}^* \to \mathcal{Q}_{S_\pm}$ is a Poisson structure and $\mathbb{K}_\pm^0 : \mathcal{Q}_{E_\pm}^* \to \mathcal{Q}_{E_\pm}$ is an Onsager operator on the state spaces $\mathcal{Q}_{S_\pm}^* \to \mathcal{Q}_{S_\pm}$ and $\mathcal{Q}_{E_\pm}^* \to \mathcal{Q}_{E_\pm}$ that allows for inhomogeneous boundary conditions

along $\Gamma$ for the state variables $w_\pm$. In a similar spirit also attention has to be paid for the entries of $\mathbb{L}_{H_\pm}$ and $\mathbb{L}^*_{H_\pm}$: the operator $\mathbb{A}^*_H : \mathcal{Q}^*_w \to \mathcal{Q}^*_{H,w}$ acts on the dual of the state space $\mathcal{Q}_w$ which can accomodate inhomogeneous boundary conditions. Elements $\delta_{w_\pm} H_\pm, \mathrm{D}_{w_\pm} H_\pm$, or $\frac{1}{\partial_{\tau_\pm} H_\pm} * \mathrm{D}_{w_\pm} H_\pm$ represent functionals from the dual space $\mathcal{Q}^*_w$ and are thus characterized by bulk and trace terms by explicitly making use of relations (21e) and (22). In this way the bulk operators also generate a trace contribution on $\Gamma$

$$\mathbb{J}_\pm(q_{\tau_\pm}) := \left[\mathbb{L}_{S_\pm}\mathbb{J}^0_\pm\mathbb{L}^*_{S_\pm}\right]_{\Omega_\pm} + \left[\mathbb{L}_{S_\pm}\mathbb{J}^0_\pm\mathbb{L}^*_{S_\pm}\right]_{\Gamma_\pm}, \tag{49a}$$

$$\mathbb{K}_\pm(q_{\tau_\pm}) := \left[\mathbb{L}_{E_\pm}\mathbb{K}^0_\pm\mathbb{L}^*_{E_\pm}\right]_{\Omega_\pm} + \left[\mathbb{L}_{E_\pm}\mathbb{K}^0_\pm\mathbb{L}^*_{E_\pm}\right]_{\Gamma_\pm}. \tag{49b}$$

On $\Gamma$ the interfacial energy and entropy densities $E_\Gamma$, $S_\Gamma$ depend on the traces of the bulk states $\gamma_\pm q_\pm := (\gamma_\pm w_\pm, \gamma_\pm \tau_\pm)$ which we write with (18) as $q_\pm$ as well as on additional surface states $q_\Gamma := (w_\Gamma, \tau_\Gamma)$, collected in $q_{\Gamma\gamma} := (q_+, q_-, q_\Gamma)^\top$, cf. (19). In analogy to (43)–(47), using the surface density $H_\Gamma \in \{E_\Gamma, S_\Gamma\}$, we introduce for $i \in \{+, -, \Gamma\}$ with operators $\mathbb{A}_{w_i}$

$$\mathbb{L}_{H_\Gamma,i} = \begin{pmatrix} \mathbb{A}_{w_i} & 0 \\ -\frac{\delta_{w_i} H_\Gamma \circ \mathbb{A}_{w_i}}{\partial_{\tau_i} H_\Gamma} & \frac{1}{\partial_{\tau_i} H_\Gamma} \end{pmatrix}, \quad \mathbb{L}^*_{H_\Gamma,i} = \begin{pmatrix} \mathbb{A}^*_{w_i} & \mathbb{A}^*_{w_i}(-\frac{\square}{\partial_{\tau_i} H_\Gamma} * \mathrm{D}_{w_i} H_\Gamma) \\ 0 & \frac{1}{\partial_{\tau_i} H_\Gamma} \end{pmatrix}, \tag{50}$$

where we typically choose $\mathbb{A}_{w_i} = I$ the identity and define the following matrices as a cartesian product:

$$\mathbb{L}_{H_\Gamma} = \mathrm{diag}\left(\mathbb{L}_{H_\Gamma,+}, \mathbb{L}_{H_\Gamma,-}, \mathbb{L}_{H_\Gamma,\Gamma}\right), \tag{51a}$$

$$\mathbb{L}^*_{H_\Gamma} = \mathrm{diag}\left(\mathbb{L}^*_{H_\Gamma,+}, \mathbb{L}^*_{H_\Gamma,-}, \mathbb{L}^*_{H_\Gamma,\Gamma}\right). \tag{51b}$$

Similar to (46) this construction provides

$$\mathbb{L}^*_{H_\Gamma}\mathrm{D}\mathcal{H}_\Gamma \equiv \mathbb{L}^*_{H_\Gamma}\mathrm{D}H_\Gamma = (0,1,0,1,0,1)^\top, \tag{52}$$

so that the NIC (14) for the interfacial geometric operators

$$\mathbb{J}(q_{\Gamma\gamma}) := \mathbb{L}_{S_\Gamma}\mathbb{J}^0_\Gamma\mathbb{L}^*_{S_\Gamma} \quad \text{and} \quad \mathbb{K}(q_{\Gamma\gamma}) := \mathbb{L}_{E_\Gamma}\mathbb{K}^0_\Gamma\mathbb{L}^*_{E_\Gamma} \tag{53}$$

can be ensured for interfacial Poisson and Onsager operators $\mathbb{J}^0_\Gamma, \mathbb{K}^0_\Gamma : (\gamma\mathcal{Q})^* \times \mathcal{Q}^*_\Gamma \to (\gamma\mathcal{Q}) \times \mathcal{Q}_\Gamma$ with the property

$$\mathbb{J}^0_\Gamma(0,1,0,1,0,1)^\top = 0 = \mathbb{K}^0_\Gamma(0,1,0,1,0,1)^\top. \tag{54}$$

We further observe that above strategy can be extended to more general dissipative mechanisms modelled by (non-quadratic) convex dual dissipation potentials as discussed in Lemma 3.3. In this setting, NIC (14) is ensured if

$$\partial_{q_{\mathrm{B}}}\Psi^{0*}_{\mathrm{B}}(q_{\mathrm{B}}; (0,1)^\top) \ni 0 \quad \text{and} \quad \partial_{q_{\Gamma\gamma}}\Psi^{0*}_\Gamma(q_{\Gamma\gamma}; (0,1,0,1,0,1)^\top) \ni 0 \tag{55}$$

for some dual dissipation potentials $\Psi^{0*}_{\mathrm{B}}$ and $\Psi^{0*}_\Gamma$ with the properties established in Lemma 3.3. Moreover, it should be mentioned that also gradients of surface states can be taken into account in interfacial densities $E_\Gamma$, $S_\Gamma$. This is addressed in Sec. 4.

In view of [ZPT21, Sec. 3.4] and [Mie11a] and based on the afore discussion as well as on the results obtained in Sec. 3.2 the following statements can be concluded.

**Lemma 3.8** (Properties of geometric structures under transformations)**.** *Let the prerequisites of Lemmata 3.3 and 3.4 be satisfied and consider transformation operators $\mathbb{L}_{H_\pm}$ and $\mathbb{L}_{H_\Gamma}$ of the type* (45)–(48) *and* (51)*. Then the following statements hold true:*

1 *Let* $\mathbb{J}^0 = \mathbb{J}^0_{\mathrm{B}} + \mathbb{J}^0_{\Gamma}$ *be a Poisson operator in canonical form. Then the transformed operators* $\mathbb{J}_{\mathrm{B}}(q_{\tau_{\mathrm{B}}}) = \mathbb{L}_{S_{\mathrm{B}}}\mathbb{J}^0_{\mathrm{B}}\mathbb{L}^*_{S_{\mathrm{B}}}$ *and* $\mathbb{J}_{\Gamma}(q_{\tau_{\Gamma\gamma}}) = \mathbb{L}_{S_{\Gamma}}\mathbb{J}^0_{\Gamma}\mathbb{L}^*_{S_{\Gamma}}$ *are also Poisson operators. If* $\mathbb{J}^0_{\mathrm{B}}$ *and* $\mathbb{J}^0_{\Gamma}$ *have properties* (48a) *and* (54)*, then* $\mathbb{J}_{\mathrm{B}}(q_{\tau_{\mathrm{B}}})$ *and* $\mathbb{J}_{\Gamma}(q_{\tau_{\Gamma\gamma}})$ *satisfy the NIC* (14) *for* $S = S_{\mathrm{B}} + S_{\Gamma}$.

2 *Let* $\Psi^{0*} = \Psi^{0*}_{\mathrm{B}} + \Psi^{0*}_{\Gamma}$ *be a dual dissipation potential with the properties of L. 3.3, Items 1 & 2. Then the transformed potentials*

$$\Psi^*_{\mathrm{B}}(q_{\tau_{\mathrm{B}}};\xi_{\mathrm{B}}) = \Psi^{0*}_{\mathrm{B}}(\mathbb{L}^*_{E_{\mathrm{B}}}q_{\tau_{\mathrm{B}}};\mathbb{L}^*_{E_{\mathrm{B}}}\xi_{\mathrm{B}})\,, \quad \Psi^*_{\Gamma}(\mathbb{L}_{E_{\Gamma}}q_{\tau_{\Gamma\gamma}};\mathbb{L}_{E_{\Gamma}}\xi_{\Gamma\gamma}) = \Psi^{0*}_{\Gamma}(\mathbb{L}^*_{E_{\Gamma}}q_{\tau_{\Gamma\gamma}};\mathbb{L}^*_{E_{\Gamma}}\xi_{\Gamma\gamma})$$

*also have properties of L. 3.3, Items 1 & 2. If* $\Psi^{0*}_{\mathrm{B}}$ *and* $\Psi^{0*}_{\Gamma}$ *have properties* (55)*, then the transformed* $\Psi^*_{\mathrm{B}}(q_{\tau_{\mathrm{B}}})$ *and* $\Psi^*_{\Gamma}(q_{\tau_{\Gamma\gamma}})$ *satisfy the NIC* (14) *for* $E = E_{\mathrm{B}} + E_{\Gamma}$.

**Remark 3.9** (The Gibbs' relation)**.** Due to the expressions $\mathbb{L}^*_S\mathrm{D}\mathcal{E}$ and $\mathbb{L}^*_E\mathrm{D}\mathcal{S}$ arising in the above GENERIC formalism, we will deal with expressions of the form $\frac{\partial_\tau E}{\partial_\tau S}$. In case $\tau = \theta$ these expressions are covered by the so-called

$$\text{Gibbs' relation: } \frac{\partial_\theta \mathcal{S}}{\partial_\theta \mathcal{E}} = \frac{1}{\theta}\,. \tag{56}$$

Mielke [Mie11a] demonstrates the generalization $\frac{\partial_\tau \mathcal{S}}{\partial_\tau \mathcal{E}} = \frac{1}{\theta}$, which we will frequently use in Section 4 and see Example 3.10 below. ⋆

**Example 3.10** (Specific choice of driving functionals in thermoelasticity)**.** In case of $\tau = \theta$ a specific choice for the bulk and surface functionals matching with Gibbs' relation (56) is given by

$$U_{\mathrm{B}}(e,\theta) = W(e) - \phi_0(\theta) + \theta\phi_0'(\theta), \qquad S_{\mathrm{B}}(e,\theta) = \phi_0'(\theta) - \mathbb{B} : e, \tag{57a}$$

$$U_{\Gamma}(\gamma_+\theta_+,\gamma_-\theta_-) = \tfrac{1}{4}(\gamma_+\theta_+^2 + \gamma_-\theta_-^2), \qquad S_{\Gamma}(\gamma_+\theta_+,\gamma_-\theta_-) = \tfrac{1}{2}(\gamma_+\theta_+ + \gamma_-\theta_-), \tag{57b}$$

e.g., with $\phi_0'(\theta) = c_{\mathrm{V}}\ln\theta$ and a matrix $\mathbb{B} \in \mathbb{R}^{d\times d}$. Clearly, both the bulk functionals in (57a) and the surface functionals obtained by (59) satisfy Gibbs' relation (56).

For the transformation $\mathrm{T}_{\theta\to S}$ we have for the bulk terms $\tilde\theta_{\mathrm{B}} = \mathrm{T}^{-1}_{\theta\to S}(S_{\mathrm{B}}) = (\phi_0')^{-1}(S_{\mathrm{B}} + \mathbb{B} : e)$ and

$$\tilde U_{\mathrm{B}}(e,S_{\mathrm{B}}) = W(e) - \phi_0\big((\phi_0')^{-1}(S_{\mathrm{B}} + \mathbb{B} : e)\big) + \big((\phi_0')^{-1}(S_{\mathrm{B}} + \mathbb{B} : e)\big)(S_{\mathrm{B}} + \mathbb{B} : e),$$

which again results in the Gibbs' relation $\partial_{S_{\mathrm{B}}}\tilde U_{\mathrm{B}}(e,S_{\mathrm{B}}) = (\phi_0')^{-1}(S_{\mathrm{B}} + \mathbb{B} : e) = \tilde\theta_{\mathrm{B}}$. We further deduce that $\gamma_\pm\tilde\theta_\pm = 2\gamma_\pm S_\pm$ and $\tilde U_{\Gamma}(\gamma_\pm S_+,\gamma_\pm S_-) = S_+^2 + S_-^2$. This also provides the interfacial Gibbs' relation $\partial_{\gamma_\pm S_\pm}U_{\Gamma} = 2\gamma_\pm S_\pm = \gamma_\pm\tilde\theta_\pm$.

Similarly, for the transformation $\mathrm{T}_{\theta\to U}$ it is $\hat\theta_{\mathrm{B}} = \mathrm{T}^{-1}_{\theta\to U}(U_{\mathrm{B}}) = h^{-1}(U_{\mathrm{B}} - W(e))$, where we have set $h(\theta_{\mathrm{B}}) := -\phi_0(\theta) + \theta\phi_0'(\theta)$, and $\hat S_{\mathrm{B}}(e,U_{\mathrm{B}}) = \phi_0'(h^{-1}(\tilde U_{\mathrm{B}} - W(e)))$. Direct calculation again gives the Gibbs' relation for the bulk, since $\partial_{U_{\mathrm{B}}}\hat S_{\mathrm{B}}(e,U_{\mathrm{B}}) = \phi_0''(\hat\theta_{\mathrm{B}})\partial_{U_{\mathrm{B}}}\hat\theta_{\mathrm{B}}$ and $\partial_{U_{\mathrm{B}}}\hat\theta_{\mathrm{B}} = 1/h' = 1/(\hat\theta_{\mathrm{B}}\phi_0''(\hat\theta_{\mathrm{B}}))$. Along $\Gamma$ we now have $\gamma_\pm\hat\theta_\pm = 2\sqrt{\gamma_\pm U_\pm}$ and $S_{\Gamma}(\gamma_+U_+,\gamma_-U_-) = \sqrt{\gamma_+U_+} + \sqrt{\gamma_-U_-}$, so that indeed $\partial_{\gamma_\pm U_\pm}S_{\Gamma} + 1/(2\sqrt{\gamma_\pm U_\pm}) = 1/(\gamma_\pm\hat\theta_\pm)$, which confirms the interfacial Gibbs' relation also for the choice $\tau = U$. Since $E = E_{\mathrm{kin}} + U$ the same calculations also verify Gibbs' relation for $\tau = E$. ⋆

# 4 Delamination processes in thermoviscoelastic materials

We now consider a composite consisting of two thermo-viscoelastic bodies glued together along the interface $\Gamma$ by an elastic adhesive. This adhesive can experience damage, in other words, delamination

may evolve along $\Gamma$. In the spirit of generalized standard materials [HN75] this process is modeled with the aid of an internal variable, the delamination variable $z : [0,\mathsf{T}] \times \Gamma \to [0,1]$ solely defined on $\Gamma$ to account for the degradation state of the glue. In particular, $z(t,x) = 1$ means that the glue is fully intact in the interfacial point $x \in \Gamma$ at time $t \in [0,\mathsf{T}]$, whereas $z(t,x) = 0$ means that the glue is completely broken in $(t,x) \in [0,\mathsf{T}] \times \Gamma$. In this way $z$ indicates the degradation state of the glue and in particular the set $\mathrm{C}(t) := \{x \in \Gamma,\, z(t,x) = 0\}$ describes the crack set. This meaning of $z$ is connected to adhesive delamination and brittle fracture processes in the sense of Griffith [Gri21], see e.g. also [Fré02], rather than to so-called cohesive zone models in the sense of Barenblatt [Bar62]. For the latter type of models the internal variable has a different meaning as it is introduced to keep track of the history of displacement jumps across $\Gamma$, for example in the form $z(t,x) := \max_{s\in[0,t]} [\![u(s,x)]\!]\cdot \mathrm{n}$. We refer to [Tho17, TZ17] for a comparison of these different types of modeling approaches and to the references therein for an analytical treatment of cohesive zone models in absence of thermal effects.

**The state vector.** The vector of bulk state variables is given by $q_{\mathrm{B}} := (u,p,\tau)$ the displacements $u : \Omega\backslash\Gamma \to \mathbb{R}^d$, the momentum $p = \varrho\dot{u} : \Omega\backslash\Gamma \to \mathbb{R}^d$ with given mass density $\varrho > 0$, and a thermodynamic state variable $\tau : \Omega\backslash\Gamma \to \mathbb{R}$ with $\tau \in \{E,S,U,\theta\}$, where we omit the index $_{\mathrm{B}}$ on the individual variables. Along $\Gamma$ we have the traces $u_\pm, p_\pm$, and $\tau_\pm$ and the surface state variables, the delamination variable $z$ and the interfacial thermodynamic variable $\tau_\Gamma$. Hence, writing $w := (u,p)$, the vector of interfacial variables is composed by

$$q_{\Gamma\gamma} = \gamma q_{\mathrm{B}} = (w_+,\tau_+,w_-,\tau_-,z,\tau_\Gamma)^\top = (u_+,p_+,\tau_+,u_-,p_-,\tau_-,z,\tau_\Gamma)^\top , \tag{58}$$

**Prototypic driving functionals.** This choice of variables is complemented by an ansatz for the potentials of the form

$$\begin{aligned}
E_{\mathrm{B}}(q_{\mathrm{B}}) &:= \tfrac{1}{2\varrho}|p|^2 + U_{\mathrm{B}}(e(u),\tau) - f\cdot u && \text{in } \Omega\backslash\Gamma, && (59a)\\
U_{\mathrm{B}}(e(u),\tau) &:= U_{\mathrm{B}}^{\mathrm{el}}(e(u)) + U_{\mathrm{B}}^{\mathrm{th}}(\tau) && \text{in } \Omega\backslash\Gamma, && (59b)\\
S_{\mathrm{B}}(q_{\mathrm{B}}) &:= S_{\mathrm{B}}^{\mathrm{th}}(e(u),\tau) && \text{in } \Omega\backslash\Gamma, && (59c)\\
E_\Gamma(\gamma q_{\mathrm{B}}) &:= \tfrac{1}{2}\big(\gamma_+ U_{\mathrm{B}}^{\mathrm{th}}(\tau) + \gamma_- U_{\mathrm{B}}^{\mathrm{th}}(\tau)\big) + U_\Gamma^{\mathrm{el}}(z,[\![u]\!]) + U_\Gamma^{\mathrm{th}}(\tau_\Gamma) && \text{on } \Gamma, && (59d)\\
S_\Gamma(\gamma q_{\mathrm{B}}) &:= \tfrac{1}{2}\big(\gamma_+ S_{\mathrm{B}}^{\mathrm{th}}(\tau) + \gamma_- S_{\mathrm{B}}^{\mathrm{th}}(\tau)\big) + S_\Gamma^{\mathrm{th}}(\tau_\Gamma) && \text{on } \Gamma, && (59e)
\end{aligned}$$

where $e(u) := \frac{1}{2}(\nabla u + \nabla u^\top)$ is the linearized strain tensor and $[\![u]\!]$ is the displacement jump as introduced in Def. 3.1. We assume that the Gibbs' relation is satisfied both in the bulk and on the interface, i.e.,

$$\frac{\partial_\tau E_{\mathrm{B}}}{\partial_\tau S_{\mathrm{B}}} = \theta_{\mathrm{B}}\,, \quad \frac{\partial_{\tau_\Gamma} E_\Gamma}{\partial_{\tau_\Gamma} S_\Gamma} = \theta_\Gamma \quad \text{and} \quad \frac{\partial_{\tau_\pm} E_\Gamma}{\partial_{\tau_\pm} S_\Gamma} = \gamma_\pm\theta_\pm\,, \tag{60}$$

see also Example 3.10 below for a specific choice matching with (60).

**Underlying Poisson and Onsager structures.** We introduce the bulk Poisson operator and bulk dual dissipation potential

$$\mathbb{J}_{\mathrm{B}}^0 := \begin{pmatrix} 0 & I & 0\\ -I & 0 & 0\\ 0 & 0 & 0\end{pmatrix} \quad \text{and} \quad \Psi_{\mathrm{B}}^{0*}(q_{\mathrm{B}};\xi_{\mathrm{B}}) := \Psi_{\mathrm{V}}^{0*}(q_{\mathrm{B}};\xi_p) + \Psi_{\mathrm{H}}^{0*}(q_{\mathrm{B}};\xi_\tau)\,. \tag{61a}$$

Here, $\mathbb{J}_{\mathrm{B}}^0$ features the reversible contribution to the evolution of the pair $(u,p)$, whereas the bulk thermodynamic variable $\tau$ evolves solely dissipative and thus has no non-zero entries in $\mathbb{J}_{\mathrm{B}}^0$. In this way, there clearly holds $\mathbb{J}_{\mathrm{B}}^0(0,0,1)^\top = 0$, as a prerequisite to satisfy NIC according to (48). In turn,

the dissipative evolution of $\tau$ is ruled by the dual dissipation potential $\Psi^*_{\mathrm{H}}(q_{\mathrm{B}};\xi_\tau)$ with density $\psi^*_{\mathrm{H}}$ of the form

$$\Psi^{0*}_{\mathrm{H}}(\theta;\xi_\tau) := \int_{\Omega\setminus\Gamma} \tfrac{\theta^2\kappa(\theta)}{2}\big|\nabla\xi_\tau\big|^2\,\mathrm{d}x\,, \tag{61b}$$

resulting in the bulk Onsager operator for heat transport

$$\mathbb{K}^0_{\mathrm{H_B}}(\theta)\xi_{\tau_{\mathrm{B}}} = \sum_{i\in\{+,-\}}\Big[-\operatorname{div}\big(\theta^2\kappa(\theta)\nabla\xi_\tau\big)\Big]_{\Omega_i} + \Big[\gamma_i\big(\theta^2\kappa(\theta)\nabla\xi_\tau\big)\mathrm{n}_i\Big]_{\Gamma_i}\,. \tag{61c}$$

This operator satisfies $\mathbb{K}^0_{\mathrm{H_B}}(\theta)1 = 0$, a prerequisite to satisfy the NIC (48). In addition, the bulk dual dissipation potential features Kelvin-Voigt viscosity of the form

$$\Psi^{0*}_{\mathrm{V}}(q_{\mathrm{B}};\xi_p) := \int_{\Omega\setminus\Gamma}\frac{1}{2}\mathbb{D}(q_{\mathrm{B}})\xi_p : \xi_p\,\mathrm{d}x \tag{61d}$$

$$\text{with}\quad \mathbb{K}^0_{\mathrm{V}}(q_{\mathrm{B}})\xi_p := \sum_{i\in\{+,-\}}\Big[\mathbb{D}(q_{\mathrm{B}})\xi_p\Big]_{\Omega_i}\,, \tag{61e}$$

the viscous Onsager operator. The full bulk Onsager operator is thus given as

$$\mathbb{K}^0_{\mathrm{B}}(q_{\mathrm{B}}) = \operatorname{diag}\big(0,\,\mathbb{K}^0_{\mathrm{V}}(q_{\mathrm{B}}),\,\mathbb{K}^0_{\mathrm{H_B}}(\theta)\big)\,. \tag{61f}$$

On the interface $\Gamma$ dissipation occurs due to heat exchange between $\Omega_\pm$ and $\Gamma$. Writing $\xi_{\gamma\tau} = (\xi_{\tau+},\xi_{\tau-},\xi_{\tau\Gamma})$ the dissipation for imperfect heat transfer has the general form

$$\begin{aligned}\Psi^{0*}_{\mathrm{H}\Gamma}(\theta_\gamma;\xi_{\gamma\tau}) &:= \int_\Gamma \tfrac{1}{2}\,\xi_{\gamma\tau}\cdot\hat\kappa_\Gamma(\theta_+,\theta_-,\theta_\Gamma)\,\xi_{\gamma\tau}\,\mathrm{d}\mathcal{H}^{d-1}\,,\\ \text{where } \hat\kappa_\Gamma &:= \begin{pmatrix}\kappa_{\Gamma,++} & \kappa_{\Gamma,+-} & \kappa_{\Gamma,+\Gamma}\\ \kappa_{\Gamma,-+} & \kappa_{\Gamma,--} & \kappa_{\Gamma,-\Gamma}\\ \kappa_{\Gamma,\Gamma+} & \kappa_{\Gamma,\Gamma-} & \kappa_{\Gamma,\Gamma\Gamma}\end{pmatrix}\ \text{such that}\ \hat\kappa_\Gamma\begin{pmatrix}1\\1\\1\end{pmatrix} = 0\,,\end{aligned} \tag{62}$$

and $\hat\kappa_\Gamma$ is positive semidefinite. We additionally account for dissipation due to processes involving $z$ on the interface by the dual dissipation potential

$$\mathcal{R}^*_z(q_\Gamma,\xi_z) := \int_\Gamma R^*_{\mathrm{D}}(q_\Gamma,\xi_z)\,\mathrm{d}\mathcal{H}^{d-1}\,, \tag{63}$$

where for fixed $q_\Gamma$ the function $\xi_z \mapsto R^*_{\mathrm{D}}(q_\Gamma,\xi_z)$ is convex and lower semicontinuous, see Sec. 4.2 for more details. Writing $\eta(\cdot) := \eta(q_\Gamma,\cdot) = \partial_{\xi_z}R^*_{\mathrm{D}}(q_\Gamma,\cdot)$ we find the following form of $\mathbb{K}^0_\Gamma$ with entries $\kappa_{\Gamma,ij}$ from (62) for $i,j\in\{+,-,\Gamma\}$

$$\mathbb{K}^0_\Gamma := \begin{pmatrix}0&0&0&0&0&0\\ 0&\kappa_{\Gamma,++}&0&\kappa_{\Gamma,+-}&0&\kappa_{\Gamma,+\Gamma}\\ 0&0&0&0&0&0\\ 0&\kappa_{\Gamma,-+}&0&\kappa_{\Gamma,--}&0&\kappa_{\Gamma,-\Gamma}\\ 0&0&0&0&\eta(\square)&0\\ 0&\kappa_{\Gamma,\Gamma+}&0&\kappa_{\Gamma,\Gamma-}&0&\kappa_{\Gamma,\Gamma\Gamma}\end{pmatrix}\,, \tag{64}$$

where the first and the third line collect the entries for $\xi_{w_\pm}$ with $w=(u,p)$. Again, we confirm that $\mathbb{K}^0_\Gamma(0,1,0,1,0,1)^\top = 0$ as a prerequisite for NIC by (54).

Since the interface functionals in (59) account for a mutual interaction of the traces of $w$ (i.e. of $u$), there is a conservative contribution to the evolution along $\Gamma$ and hence we set

$$\mathbb{J}^0_{\mathrm{HD}_\Gamma} := \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{65}$$

**Noninteraction conditions** (14)**.** In order to ensure the NIC (14) we follow the approach of Sec. 3.4 to find the Poisson structures $\mathbb{J}_{\mathrm{B}}, \mathbb{J}_\Gamma$ and the Onsager operators $\mathbb{K}_{\mathrm{B}}, \mathbb{K}_\Gamma$. In particular, we introduce the bulk Poisson structure according to (49) and (45) in the specific form

$$\mathbb{J}_{\mathrm{B}}(q_\tau) = \mathbb{L}_{S_{\mathrm{B}}} \mathbb{J}^0_{\mathrm{B}} \mathbb{L}^*_{S_{\mathrm{B}}}, \quad \text{where} \quad \mathbb{L}^*_{S_{\mathrm{B}}} = \begin{pmatrix} I & 0 & -\frac{\square}{\partial_\tau S_{\mathrm{B}}} * \mathrm{D}_u S_{\mathrm{B}} \\ 0 & I & -\frac{\square}{\partial_\tau S_{\mathrm{B}}} * \mathrm{D}_p S_{\mathrm{B}} \\ 0 & 0 & \frac{1}{\partial_\tau S_{\mathrm{B}}} \end{pmatrix} \tag{66a}$$

$$\text{with } \delta_p S_{\mathrm{B}} = (0, \dots, 0), \text{ and } \mathrm{D}_p S_{\mathrm{B}} = (0, \dots, 0)^\top \in \mathbb{R}^d$$

$$\text{and } -\tfrac{\square}{\partial_\tau S_{\mathrm{B}}} * \mathrm{D}_u S_{\mathrm{B}} = \sum_{i \in \{+,-\}} \big[\mathrm{div}\big(\tfrac{\square}{\partial_\tau S_{\mathrm{B}}} \partial_e S_{\mathrm{B}}\big)\big]_{\Omega_i} - \big[\gamma_i\big(\tfrac{\square}{\partial_\tau S_{\mathrm{B}}} \partial_e S_{\mathrm{B}}\big)\mathrm{n}_i\big]_{\Gamma_i}, \tag{66b}$$

so that this entry in $\mathbb{L}^*_{S_{\mathrm{B}}}$ also generates a non-zero trace contribution on $\Gamma_\pm$. It can be readily checked that $\mathbb{L}^*_{S_{\mathrm{B}}} \mathrm{D} S_{\mathrm{B}} = (0,0,1)^\top$, which ensures the NIC (14) $\mathbb{J}_{\mathrm{B}}(q_{\tau_{\mathrm{B}}}) \mathrm{D} S_{\mathrm{B}} = \mathbb{L}_{S_{\mathrm{B}}} \mathbb{J}^0_{\mathrm{B}} \mathbb{L}^*_{S_{\mathrm{B}}} \mathrm{D} S_{\mathrm{B}} = 0$ by the form of $\mathbb{J}^0_{\mathrm{B}}$ from (61a).

For the bulk Onsager contribution we also follow (47) and (45), i.e.,

$$\mathbb{K}_{\mathrm{B}}(q_\tau) = \mathbb{L}_{E_{\mathrm{B}}} \mathbb{K}^0_{\mathrm{B}} \mathbb{L}^*_{E_{\mathrm{B}}}, \quad \text{where} \quad \mathbb{L}^*_{E_{\mathrm{B}}} = \begin{pmatrix} I & 0 & -\frac{\square}{\partial_\tau E_{\mathrm{B}}} * \mathrm{D}_u E_{\mathrm{B}} \\ 0 & e(\square) & e \circ \Big(-\frac{\square}{\partial_\tau E_{\mathrm{B}}} * \mathrm{D}_p E_{\mathrm{B}}\Big) \\ 0 & 0 & \frac{1}{\partial_\tau E_{\mathrm{B}}} \end{pmatrix} \tag{66c}$$

$$\begin{aligned} &\text{with } \delta_p E_{\mathrm{B}} = \partial_p E_{\mathrm{B}}^\top = p/\varrho, \\ &\quad -\tfrac{\square}{\partial_\tau E_{\mathrm{B}}} * \mathrm{D}_u E_{\mathrm{B}} = \sum_{i \in \{+,-\}} \big[\mathrm{div}\big(\tfrac{\square}{\partial_\tau E_{\mathrm{B}}} \partial_e E_{\mathrm{B}}\big)\big]_{\Omega_i} - \big[\big(\tfrac{\square}{\partial_\tau E_{\mathrm{B}}} \partial_e E_{\mathrm{B}}\big)\mathrm{n}_i\big]_{\Gamma_i}, \\ &\text{and } e^*(\xi_p) = \sum_{i \in \{+,-\}} \big[-\mathrm{div}\,\xi_p\big]_{\Omega_i} + \big[\gamma_i \xi_p \cdot \mathrm{n}_i\big]_{\Gamma_i}. \end{aligned} \tag{66d}$$

Comparing with (45) this means that here $\mathbb{A}_H = e^*$. The operators $e$, $e^*$ together with the viscous Onsager operator $\mathbb{K}^0_{\mathrm{V}}$ generate the dissipative contributions for Kelvin-Voigt viscoelasticity.

Similarly, the interfacial geometric structures $\mathbb{J}_\Gamma$ and $\mathbb{K}_\Gamma$ are deduced according to (48) by transforming $\mathbb{K}^0_\Gamma$ and $\mathbb{J}^0_\Gamma$ using the transformation maps $\mathbb{L}_{E_\Gamma}, \mathbb{L}^*_{E_\Gamma}$ as well as $\mathbb{L}_{S_\Gamma}, \mathbb{L}^*_{S_\Gamma}$ obtained by (51).

**Elimination of surface thermodynamic variable $\tau_\Gamma$ by local equilibrium.** We specify $\hat\kappa_\Gamma$ from (62) as

$$\hat\kappa_\Gamma(\theta_\gamma) = \kappa_\Gamma(\theta_\gamma) \begin{pmatrix} 1+\frac{1}{4\epsilon} & -1+\frac{1}{4\epsilon} & -\frac{1}{2\epsilon} \\ -1+\frac{1}{4\epsilon} & 1+\frac{1}{4\epsilon} & -\frac{1}{2\epsilon} \\ -\frac{1}{2\epsilon} & -\frac{1}{2\epsilon} & \frac{1}{\epsilon} \end{pmatrix},$$

$$\text{i.e.} \quad \xi \cdot \hat\kappa_\Gamma \xi = \kappa_\Gamma(\xi_{\tau+} - \xi_{\tau-})^2 + \epsilon^{-1}(\xi_{\tau\Gamma} - \tfrac{1}{2}(\xi_{\tau+} + \xi_{\tau-}))^2$$

and consider $\mathbb{K}_\Gamma = \mathbb{L}_{S_\Gamma}\mathbb{K}^0_\Gamma\mathbb{L}^*_{S_\Gamma}$ with $\mathbb{K}^0_\Gamma$ from (64). Using the Gibbs' relation $\frac{\partial_{\tau i}S_\Gamma}{\partial_{\tau i}E_\Gamma} = \theta_i^{-1}$ for $i \in \{+,-,\Gamma\}$ we calculate the entries of $\mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma$ as follows

$$
\begin{aligned}
(\mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma)_{w_+} &= (\mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma)_{w-} = 0\,,\\
(\mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma)_{\tau_\pm} &= \kappa_\Gamma \tfrac{1}{\partial_{\tau_\pm}E_\Gamma}\left((\theta_\pm^{-1}-\theta_\mp^{-1}) - \frac{1}{2\epsilon}\left(\theta_\Gamma^{-1} - \tfrac{1}{2}(\theta_+^{-1}+\theta_-^{-1})\right)\right)\\
(\mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma)_{z} &= \eta\left(\partial_z S_\Gamma - \theta_\Gamma^{-1} * \partial_z E_\Gamma\right)\\
(\mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma)_{\tau_\Gamma} &= -\tfrac{1}{\partial_{\tau_\Gamma}E_\Gamma}\eta\left(\partial_z S_\Gamma - \theta_\Gamma^{-1} * \partial_z E_\Gamma\right) + \tfrac{1}{\partial_{\tau_\Gamma}E_\Gamma}\frac{\kappa_\Gamma}{\epsilon}\left(\theta_\Gamma^{-1} - \tfrac{1}{2}(\theta_+^{-1}+\theta_-^{-1})\right)
\end{aligned}
$$

Under the assumption that the system is quasi-stationary with respect to $\tau_\Gamma$ we have $(\mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma)_{\tau_\Gamma} = 0$ and hence in the second row:

$$
(\mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma)_{\tau_\pm} = \kappa_\Gamma \tfrac{1}{\partial_{\tau_\pm}E_\Gamma}\left((\theta_\pm^{-1}-\theta_\mp^{-1})\right) - \tfrac{1}{2\,\partial_{\tau_\pm}E_\Gamma}\eta\left(\partial_z S_\Gamma - \theta_\Gamma^{-1} * \partial_z E_\Gamma\right)\,.
$$

The last expression cannot yet be rephrased in terms of a gradient flow. However, the limit $\epsilon \to 0$ formally enforces that $\frac{1}{\theta_\Gamma} \approx \frac{1}{2}(\frac{1}{\theta_+} + \frac{1}{\theta_-})$. Then we find the new GENERIC system by eliminating the row for $\tau_\Gamma$ in $\mathbb{K}^0_\Gamma$ and $\mathbb{J}^0_\Gamma$ in (64) and (65) by and modifying $\mathbb{L}_{E_\Gamma}$ and $\mathbb{L}^*_{E_\Gamma}$ in the following way

$$
\mathbb{L}_{E_\Gamma} = \begin{pmatrix}
I_{w_+} & 0 & 0 & 0 & 0\\
-\frac{1}{\partial_{\tau_+}E_\Gamma}\delta_{w_+}E_\Gamma & \frac{1}{\partial_{\tau_+}E_\Gamma} & 0 & 0 & -\frac{1}{2\,\partial_{\tau_+}E_\Gamma}\delta_z E_\Gamma\\
0 & 0 & I_{w_-} & 0 & 0\\
0 & 0 & -\frac{1}{\partial_{\tau_-}E_\Gamma}\delta_{w_-}E_\Gamma & \frac{1}{\partial_{\tau_-}E_\Gamma} & -\frac{1}{2\,\partial_{\tau_-}E_\Gamma}\delta_z E_\Gamma\\
0 & 0 & 0 & 0 & I_z
\end{pmatrix}, \tag{67a}
$$

$$
\mathbb{L}^*_{E_\Gamma} = \begin{pmatrix}
I_{w_+} & -\frac{\square}{\partial_{\tau_+}E_\Gamma} * \mathrm{D}_{w_+}E_\Gamma & 0 & 0 & 0\\
0 & \frac{1}{\partial_{\tau_+}E_\Gamma} & 0 & 0 & 0\\
0 & 0 & I_{w_-} & -\frac{\square}{\partial_{\tau_-}E_\Gamma} * \mathrm{D}_{w_-}E_\Gamma & 0\\
0 & 0 & 0 & \frac{1}{\partial_{\tau_-}E_\Gamma} & 0\\
0 & -\frac{\square}{2\,\partial_{\tau_+}E_\Gamma} * \mathrm{D}_z E_\Gamma & 0 & -\frac{\square}{2\,\partial_{\tau_-}E_\Gamma} * \mathrm{D}_z E_\Gamma & I_z
\end{pmatrix}. \tag{67b}
$$

and similarly for $\mathbb{L}_{S_\Gamma}$ and $\mathbb{L}^*_{S_\Gamma}$

**Weak formulation of the GENERIC system with bulk-interface coupling.** Altogether, the weak formulation of the GENERIC evolution system

$$
\langle \tilde{\xi}, \dot{q}\rangle_{\mathcal{Q}} = \langle \tilde{\xi}, \mathbb{J}_{\mathrm{B}}\mathrm{D}\mathcal{E}_{\mathrm{B}} + \mathbb{K}_{\mathrm{B}}\mathrm{D}\mathcal{S}_{\mathrm{B}}\rangle_{\mathcal{Q}_{\mathrm{B}}} + \langle \tilde{\xi}_{\Gamma\gamma}, \mathbb{J}_\Gamma \mathrm{D}\mathcal{E}_\Gamma + \mathbb{K}_\Gamma \mathrm{D}\mathcal{S}_\Gamma\rangle_{\mathcal{Q}_\Gamma} \tag{68}
$$

for all admissible test functions $\tilde{\xi} = (\tilde{\xi}_{\mathrm{B}}, \tilde{\xi}_z) = (\tilde{\xi}_u, \tilde{\xi}_p, \tilde{\xi}_\tau, \tilde{\xi}_z) \in \mathcal{Q}^*$ and the interfacial test functions $\tilde{\xi}_{\Gamma\gamma} = (\gamma_+\tilde{\xi}_{\mathrm{B}}, \gamma_-\tilde{\xi}_{\mathrm{B}}, \tilde{\xi}_z) \in \mathcal{Q}^*_{\Gamma\gamma}$ can be written as follows when collecting terms that use the same

test function

$$\begin{aligned}
\langle\tilde{\xi}_u,\dot{u}\rangle_{\mathcal{Q}_u} &= \langle\tilde{\xi}_u,p/\varrho\rangle_{\mathcal{Q}_u}\,, && \text{(69a)}\\
\langle\tilde{\xi}_p,\dot{p}\rangle_{\mathcal{Q}_p} &= \langle\tilde{\xi}_p,\operatorname{div}(\partial_e W(e(u))+\mathbb{D}e(\dot{u})-\tfrac{\partial_\tau E_{\mathrm{B}}}{\partial_\tau S_{\mathrm{B}}}\partial_e S_{\mathrm{B}})+f\rangle_{\Omega\setminus\Gamma}\\
&\quad+\sum_{i\in\{+,-\}}-\langle\gamma_i\tilde{\xi}_p,\gamma_i\big(\partial_e W_{\mathrm{B}}(e(u))+\mathbb{D}e(\dot{u})-\tfrac{\partial_\tau E_{\mathrm{B}}}{\partial_\tau S_{\mathrm{B}}}\partial_e S_{\mathrm{B}}\big)\mathrm{n}_i\rangle_{\Gamma_i}\\
&\quad+\langle\gamma_i\tilde{\xi}_p,\partial_{\gamma_i u}U_\Gamma^{\mathrm{el}}(z,[\![u]\!])\rangle_\Gamma\,, && \text{(69b)}\\
\langle\tilde{\xi}_z,\dot{z}\rangle_{\mathcal{Q}_z} &= \langle\tilde{\xi}_z,\eta_z\rangle_{\mathcal{Q}_z}\ \text{and}\ \eta_z\in\partial_{\xi_z}R_{\mathrm{D}}^*\big(q_{\Gamma\gamma};-\tfrac12\big(\tfrac{1}{\theta_+}+\tfrac{1}{\theta_-}\big)*\mathrm{D}_z U_\Gamma^{\mathrm{el}}(z,[\![u]\!])\big)\,, && \text{(69c)}\\
\langle\tilde{\xi}_\tau,\dot{\tau}\rangle_{\mathcal{Q}_\tau} &= \langle\tfrac{\tilde{\xi}_\tau}{\partial_\tau E_{\mathrm{B}}},-\operatorname{div}\Big(\kappa(\theta)\nabla\tfrac{\partial_\tau S_{\mathrm{B}}}{\partial_\tau E_{\mathrm{B}}}\Big)-\tfrac{\partial_\tau E_{\mathrm{B}}}{\partial_\tau S_{\mathrm{B}}}\partial_e S_{\mathrm{B}}:e(\dot{u})+e(\dot{u}):\mathbb{D}e(\dot{u})\rangle_{\Omega\setminus\Gamma}\\
&\quad+\sum_{i\in\{+,-\}}\langle\gamma_i\big(\tfrac{\tilde{\xi}_\tau}{\partial_\tau E_{\mathrm{B}}}\big),\gamma_i\big(\kappa(\theta)\nabla\tfrac{\partial_\tau S_{\mathrm{B}}}{\partial_\tau E_{\mathrm{B}}}\big)\mathrm{n}_i\rangle_{\Gamma_i}+\langle\gamma_i\tilde{\xi}_\tau,-\tfrac{1}{2\partial_{\gamma_i\tau}E_\Gamma}\delta_z U_\Gamma^{\mathrm{el}}\cdot\eta_z\rangle_\Gamma\\
&\quad+\langle\big(\tfrac{\gamma_+\tilde{\xi}_\tau}{\partial_{\gamma_+\tau}E_\Gamma}-\tfrac{\gamma_-\tilde{\xi}_\tau}{\partial_{\gamma_-\tau}E_\Gamma}\big),\kappa_\Gamma([\![u]\!],z)[\![\theta]\!]\rangle_\Gamma\,, && \text{(69d)}
\end{aligned}$$

where $\eta_z=\dot{z}\in\partial_{\xi_z}R_{\mathrm{D}}^*\big(q_{\Gamma\gamma};-\frac12\big(\frac{1}{\theta_+}+\frac{1}{\theta_-}\big)*\mathrm{D}_z U_\Gamma^{\mathrm{el}}\big)$ by (69c). Using for the test functions in (69d) the ansatz $\tilde{\xi}_\tau=\partial_\tau E_{\mathrm{B}}\hat{\xi}_\tau$ for any suitable $\hat{\xi}_\tau$ and exploiting the Gibbs' relation, equation (69d) can be rewritten as

$$\begin{aligned}
\langle\partial_\tau E_{\mathrm{B}}\hat{\xi}_\tau,\dot{\tau}\rangle_{\mathcal{Q}_\tau} &= \langle\hat{\xi}_\tau,-\operatorname{div}\big(\kappa(\theta)\nabla\tfrac{1}{\theta}\big)-\theta\partial_e S_{\mathrm{B}}:e(\dot{u})+e(\dot{u}):\mathbb{D}e(\dot{u})\rangle_{\Omega\setminus\Gamma}\\
&\quad+\sum_{i\in\{+,-\}}\langle\gamma_i\hat{\xi}_\tau,\gamma_i\big(\kappa(\theta)\nabla\tfrac{1}{\theta}\big)\mathrm{n}_i\rangle_{\Gamma_i}+\langle\gamma_i\hat{\xi}_\tau,-\tfrac12\delta_z U_\Gamma^{\mathrm{el}}\cdot\dot{z}\rangle_\Gamma+\langle[\![\hat{\xi}_\tau]\!],\kappa_\Gamma[\![\theta]\!]\rangle_\Gamma
\end{aligned}$$

for all suitable test functions $\hat{\xi}_\tau$. This entails the condition

$$\sum_{i\in\{+,-\}}\langle\gamma_i\hat{\xi}_\tau,\gamma_i\big(\kappa(\theta)\nabla\tfrac{1}{\theta}\big)\mathrm{n}_i\rangle_{\Gamma_i}+\langle\gamma_i\hat{\xi}_\tau,-\tfrac12\delta_z U_\Gamma^{\mathrm{el}}\cdot\dot{z}\rangle_\Gamma+\langle[\![\hat{\xi}_\tau]\!],\kappa_\Gamma[\![\theta]\!]\rangle_\Gamma=0\,. \tag{70}$$

**Derivation of interfacial coupling conditions.** From this we are now going to derive interfacial coupling conditions in strong form. For shorter notation we here set $J:=\kappa(\theta)\nabla\frac{1}{\theta}$ and with the relation $\mathrm{n}_-=-\mathrm{n}_+$ we calculate

$$\begin{aligned}
\sum_{i\in\{+,-\}}\langle\gamma_i\hat{\xi}_\tau,\gamma_i\big(\kappa(\theta)\nabla\tfrac{1}{\theta}\big)\mathrm{n}_i\rangle_{\Gamma_i} &= \langle\gamma_+\hat{\xi}_\tau,\gamma_+J\mathrm{n}_+\rangle_\Gamma-\langle\gamma_-\hat{\xi}_\tau,\gamma_-J\mathrm{n}_+\rangle_\Gamma\\
&=\langle[\![\hat{\xi}_\tau]\!],\tfrac12(\gamma_+J+\gamma_-J)\cdot\mathrm{n}_+\rangle_\Gamma+\langle\tfrac12(\gamma_+\hat{\xi}_\tau+\gamma_-\hat{\xi}_\tau),[\![J]\!]\cdot\mathrm{n}_+\rangle_\Gamma\,.
\end{aligned}$$

Comparison with the remaining terms in in (70) results in the interfacial coupling conditions (72g) and (72h) below.

Similar arguments also allow it to deduce interfacial coupling conditions from the weak momentum balance (69b): Noting that $\langle\gamma_\pm\tilde{\xi}_p,\partial_{\gamma_+u_+}U_\Gamma^{\mathrm{el}}\rangle_\Gamma=\langle-\gamma_\pm\tilde{\xi}_p,\partial_{\gamma_-u_-}U_\Gamma^{\mathrm{el}}\rangle_\Gamma$, we may rewrite the terms stemming from the interfacial energy in (69b) as follows

$$\langle\gamma_+\tilde{\xi}_p,\partial_{\gamma_+u}U_\Gamma^{\mathrm{el}}\rangle_\Gamma+\langle\gamma_-\tilde{\xi}_p,\partial_{\gamma_-u}U_\Gamma^{\mathrm{el}}\rangle_\Gamma=\langle[\![\tilde{\xi}_p]\!],\partial_{[\![u]\!]}U_\Gamma^{\mathrm{el}}\rangle_\Gamma\,.$$

Further using the abbreviation $\sigma_\pm:=\big[\partial_e W_{\mathrm{B}}(e(u))+\mathbb{D}e(\dot{u})-\frac{\partial_\tau E_{\mathrm{B}}}{\partial_\tau S_{\mathrm{B}}}\partial_e S_{\mathrm{B}}\big]_{\Omega_\pm}$ we now read from (69b) that the terms on $\Gamma$ have to satisfy the condition

$$0=\langle[\![\tilde{\xi}_p]\!],\gamma_+\sigma_+\mathrm{n}_++\partial_{[\![u]\!]}U_\Gamma^{\mathrm{el}}\rangle_\Gamma+\langle\gamma_-\tilde{\xi}_p,\gamma_+\sigma_+\mathrm{n}_++\gamma_-\sigma_-\mathrm{n}_-\rangle_\Gamma \tag{71}$$

for all test functions $\tilde{\xi}_p \in \mathcal{Q}_p^*$ with traces $\gamma_i \tilde{\xi}_p$, $i \in \{+,-\}$, and jump $[\![\tilde{\xi}_p]\!]$ across $\Gamma$. This provides the interfacial coupling conditions (72e) and (72f) below.

**Strong form of the GENERIC system with bulk-interface coupling.** From above considerations we conclude that (69) corresponds to the following strong formulation

$$\begin{aligned}
\dot{u} &= p/\varrho \quad \text{in } \Omega_\pm\,, && \text{(72a)}\\
\dot{p} &= \operatorname{div}(\partial_e U_{\mathrm{B}} + \mathbb{D}e(\dot{u}) - \theta\partial_e S_{\mathrm{B}}) + f \quad \text{in } \Omega_\pm\,, && \text{(72b)}\\
\dot{\tau} &= \tfrac{1}{\partial_\tau E_{\mathrm{B}}}\Big(\operatorname{div}(\kappa(\theta)\nabla\theta) - \theta\partial_e S_{\mathrm{B}} : e(\dot{u}) + e(\dot{u}) : \mathbb{D}e(\dot{u})\Big) \quad \text{in } \Omega_\pm\,, && \text{(72c)}\\
\dot{z} &\in \partial_{\xi_z} R_{\mathrm{D}}^*\big(q_{\Gamma\gamma}; -\tfrac{1}{2}(\tfrac{1}{\theta_+} + \tfrac{1}{\theta_-}) * \mathrm{D}_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!])\big) \quad \text{on } \Gamma\,, && \text{(72d)}
\end{aligned}$$

complemented by the following interfacial coupling conditions along $\Gamma$

$$\begin{aligned}
\gamma_+\sigma_+\mathrm{n}_+ + \gamma_-\sigma_-\mathrm{n}_- &= 0\,, && \text{(72e)}\\
\gamma_+\sigma_+\mathrm{n}_+ + \partial_{[\![u]\!]} U_\Gamma^{\mathrm{el}}(z, [\![u]\!]) &= 0\,, && \text{(72f)}\\
[\![\kappa(\theta)\nabla\tfrac{1}{\theta}]\!]\cdot\mathrm{n}_+ - \delta_z U_\Gamma^{\mathrm{el}}\cdot\dot{z} &= 0\,, && \text{(72g)}\\
\tfrac{1}{2}\big(\gamma_+(\kappa(\theta)\nabla\tfrac{1}{\theta}) + \gamma_-(\kappa(\theta)\nabla\tfrac{1}{\theta})\big)\cdot\mathrm{n}_+ + \kappa_\Gamma([\![u]\!], z)[\![\theta]\!] &= 0\,, && \text{(72h)}
\end{aligned}$$

and by homogeneous boundary conditions on $\partial\Omega$, and suitable initial conditions.

In the next sections we introduce typical choices used in mathematical literature for the dissipation potential for delamination $R_{\mathrm{D}}$ and its conjugate $R_{\mathrm{D}}^*$ in (63) and for the interfacial mechanical energy $U_\Gamma^{\mathrm{el}}$ from (59d). For these choices we discuss the resulting form of the interfacial coupling conditions (72g), (72h) and thus reveal the GENERIC structure of the models previously studied in literature with analytical methods.

## 4.1 Typical choices for interfacial mechanical energies for delamination

Interfacial mechanical energies for delamination are typically of the type

$$U_\Gamma^{\mathrm{el}}(z, [\![u]\!]) = W_\Gamma(z, [\![u]\!]) + I_{[0,1]}(z) + I_K([\![u]\!])\,. \tag{73}$$

Here, $I_{[0,1]}$ is the indicator function of the set $[0,1]$ to feature the constraint $z \in [0,1]$, i.e., $I_{[0,1]}(z) = 0$ if $z \in [0,1]$ and $I_{[0,1]}(z) = \infty$ otherwise. Moreover, the indicator function $I_K$ of the convex cone $K := \{v, [\![v]\!]\cdot\mathrm{n}_+ \geq 0\}$ ensures non-penetration of the material along the interface. Most importantly, the term $W_\Gamma(z, [\![u]\!])$ takes into account that displacement discontinuities along $\Gamma$ are energetically more costly as long as the glue is effective, i.e., for $z(t,x) > 0$. If displacement jumps are only penalised but not excluded one speaks of *adhesive contact* and a typical energy density takes the form

$$W_\Gamma^k(z, [\![u]\!]) := \frac{k}{2} z |[\![u]\!]|^2 \tag{74a}$$

with a constant $k > 0$. Displacement jumps are excluded in points where the glue active in case of *brittle delamination* with the energy density

$$W_\Gamma^\infty(z, [\![u]\!]) := I_{\mathrm{C_b}}(z, [\![u]\!]) \quad \text{with } \mathrm{C_b} := \{(\tilde{z}, [\![\tilde{u}]\!]),\ \tilde{z}|[\![\tilde{u}]\!]| = 0 \text{ a.e. on } \Gamma\} \tag{74b}$$

the set accounting for the non-smooth, *brittle constraint*. In combination with a unidirectional, rate-independent dissipation potential, cf. (76) below with $r = 1$, this provides a model for fracture in the spirit of Griffith [Gri21].

For analytical reasons some works additionally consider in $U_\Gamma^{\rm el}(z,[\![u]\!])$ a gradient term for the delamination variable. For example, [BBR09, BBR15a, BBR15b] consider the gradient term

$$G(\nabla z) := \tfrac{1}{2}|\nabla z|^2 \tag{75}$$

and [RT15] uses a Modica-Mortola type gradient term $G_{\rm M}(\nabla z) := \frac{1}{2{\rm M}}|\nabla z|^2 + \frac{\rm M}{2} z^2(1-z)^2$ to approximate as ${\rm M}\to\infty$ a model which only accounts for the fully intact $z(t,x)=1$ and the fully broken state $z(t,x)=0$. In this limit, the interfacial gradient term is given by the relative perimeter of the set $Z(t) := \{x\in\Gamma,\, z(t,x)=1\}$ in $\Gamma$.

## 4.2 Typical choices of dissipation potentials for delamination

Delamination in non-living materials is a unidirectional process, i.e., once the glue has weakened in an interfacial point it cannot heal and will ultimately break. This property can be modeled by a dissipation potential of the form

$$\begin{aligned}&\mathcal{R}_{\rm D}(q;v) := \int_\Gamma R_{\rm D}(q;v)\,{\rm d}\mathcal{H}^{d-1}\\ &\text{with } R_{\rm D}(q;v) := a(q)R_r(v) + I_{(-\infty,0]}(v) \quad \text{and } R_r(v) := \frac{1}{r}|v|^r\,,\end{aligned} \tag{76}$$

for some strictly positive, state-dependent function $a(q)>0$ for all $q$, the integrability exponent $r\in[1,\infty)$, and $I_{(-\infty,0]}$ the indicator function of the set $(-\infty,0]$, i.e., $I_{(-\infty,0]}(v)=0$ if $v\in(-\infty,0]$ and $I_{(-\infty,0]}(v)=\infty$ otherwise. Rate-independent delamination corresponds to the case $r=1$, see e.g. [RR11, RR13, RT15, RT17], while $r>1$ describes rate-dependent delamination and is most commonly treaded in literature with the exponent $r=2$, cf. e.g. [BBR15a]. When choosing $v=\dot z$ we note that the indicator function $I_{(-\infty,0]}$ in (76) entails the constraint $\dot z\le 0$, which ensures that delamination cannot heal, as $z=1$ is the intact state and $z=0$ denotes the broken state. The dual dissipation potential $\mathcal{R}_{\rm D}^*$, resp. its density $R_{\rm D}^*$, is the convex conjugate of $\mathcal{R}_{\rm D}$ obtained by (11). In the case $r=1$ this is

$$R_{\rm D}^*(q;\xi_z) = \begin{cases} 0 & \text{if } \xi_z\in[-a(q),\infty),\\ \infty & \text{otherwise,}\end{cases} \tag{77a}$$

i.e., $R_{\rm D}^*(q;\cdot) = I_{\partial_v R_{\rm D}(q;0)}$ is given by the indicator function of the convex set $\partial_v R_{\rm D}(q;0)$. For $r\in(1,\infty)$ the convex conjugate is given by

$$R_{\rm D}^*(q;\xi_z) = \begin{cases} 0 & \text{if } \xi_z>0,\\ a(q)R_{r'}\big(\frac{\xi}{a(q)}\big) & \text{otherwise,}\end{cases} \qquad \text{where } \tfrac{1}{r}+\tfrac{1}{r'}=1\,. \tag{77b}$$

We now discuss (formally) equivalent formulations for the flow rule (72d) and their implication on the coupling conditions (72g)–(72h). For this, let us first assume that $U_\Gamma^{\rm el}(z,[\![u]\!])$ is smooth and does not feature the gradient $\nabla z$. Then $\frac12\big(\frac{1}{\theta_+}+\frac{1}{\theta_-}\big)*{\rm D}_z U_\Gamma^{\rm el}(z,[\![u]\!]) = \frac12\big(\frac{1}{\theta_+}+\frac{1}{\theta_-}\big)\partial_z U_\Gamma^{\rm el}(z,[\![u]\!])$ in (72d). By convex duality, the flow rule (72d) is equivalent to the force balance

$$-\tfrac12(\tfrac{1}{\theta_+}+\tfrac{1}{\theta_-})\partial_z U_\Gamma^{\rm el}(z,[\![u]\!]) \in \partial_{\dot z} R_{\rm D}(q_{\Gamma\gamma};\dot z) \quad \text{on } \Gamma\,, \tag{78}$$

and to the Fenchel equality

$$R_{\rm D}(q_{\Gamma\gamma};\dot z) + R_{\rm D}^*\big(q_{\Gamma\gamma}; -\tfrac12(\tfrac{1}{\theta_+}+\tfrac{1}{\theta_-})\partial_z U_\Gamma^{\rm el}(z,[\![u]\!])\big) = \langle -\tfrac12(\tfrac{1}{\theta_+}+\tfrac{1}{\theta_-})\partial_z U_\Gamma^{\rm el}(z,[\![u]\!]),\dot z\rangle_\Gamma\,. \tag{79}$$

Comparing (78) with (76) we make the choice

$$a(q) := \tfrac12(\tfrac{1}{\theta_+}+\tfrac{1}{\theta_-}), \tag{80}$$

so that (78) results in the state-independent force balance

$$-\partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!]) \in \partial_{\dot z}\big(R_r(\dot z) + I_{(-\infty,0]}(\dot z)\big)\,. \tag{81}$$

This type of force balance featuring a dissipation potential independent of $\theta$ is e.g. considered in [RR11, RT15] for $r = 1$ and in [BBR09, BBR15a, BBR15b] for $r = 2$. Of course, the choice (80) also specifies $a(q) = \frac{1}{2}(\frac{1}{\theta_+} + \frac{1}{\theta_-})$ in (77b). With this ansatz, by formally dividing (79) by $a(q)$, coupling condition (72g) can be further rewritten as

$$[\![\kappa(\theta)\nabla\tfrac{1}{\theta}]\!] + R_r(\dot z) + \tfrac{1}{a(q)} R_{\mathrm{D}}^*\big(q; -\tfrac{1}{2}(\tfrac{1}{\theta_+} + \tfrac{1}{\theta_-})\partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!])\big) = 0\,. \tag{82}$$

In the rate-independent case $r = 1$, when taking into account that

$$R_{\mathrm{D}}^*(q; -\tfrac{1}{2}(\tfrac{1}{\theta_+} + \tfrac{1}{\theta_-})\partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!])) = 0$$

by (77a) and (72d), we find for (82) in particular

$$[\![\kappa(\theta)\nabla\tfrac{1}{\theta}]\!] + R_1(\dot z) + I_{(-\infty,0]}(\dot z) = 0\,. \tag{83a}$$

Moreover, in the rate-dependent case $r > 1$ it is $R_{\mathrm{D}}^*\big(q; -\frac{1}{2}(\frac{1}{\theta_+} + \frac{1}{\theta_-})\partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!])\big) = a(q) R_{r'}\big(-\partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!])\big)$ by (77b) given that $\partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!]) \geq 0$, and hence (82) provides

$$[\![\kappa(\theta)\nabla\tfrac{1}{\theta}]\!] + R_r(\dot z) + I_{(-\infty,0]}(\dot z) + R_{r'}\big(-\partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!])\big) = 0\,. \tag{83b}$$

In (73)–(74) it was discussed that mechanical energies for adhesive contact and brittle delamination for modeling reasons in general feature non-smooth but convex terms. Thus, $\partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!])$ in (78)–(83) indeed is the subdifferential of a convex function.

Now we turn to the case that $U_\Gamma^{\mathrm{el}}$ from (73) additionally also contains a quadratic gradient term $G$ as in (75). Then

$$a(q) * \mathrm{D}_z\Big(U_\Gamma^{\mathrm{el}}(z, [\![u]\!]) + G(\nabla z)\Big) = a(q)\zeta_z + \operatorname{div} a(q)\nabla z \quad \text{with } \zeta_z \in \partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!]) \tag{84}$$

in (72d). Thus the ansatz (76) and repeating above calculations does not help to remove $a(q)$ from the divergence-term. In order to find for the delamination variable a force balance that is independent of $a(q)$, one rather has to modify the ansatz used to ensure the NIC for $z$ in $\mathbb{L}_{E_\Gamma}$ and $\mathbb{L}_{E_\Gamma}^*$, see (67). More precisely, in the fifth line of $\mathbb{L}_{E_\Gamma}^*$ we replace

$$-\tfrac{\square}{2\partial_{\tau_\pm} E_\Gamma} * \mathrm{D}_z E_\Gamma \quad \text{by} \quad -\tfrac{\square}{2\partial_{\tau_\pm} E_\Gamma}\mathrm{D}_z E_\Gamma\,, \tag{85}$$

which is

$$-\tfrac{\square}{2\partial_{\tau_\pm} E_\Gamma}\mathrm{D}_z E_\Gamma = -\tfrac{\square}{2\partial_{\tau_\pm} E_\Gamma}\big(\zeta_z - \Delta_\Gamma z\big) \quad \text{with } \zeta_z \in \partial_z U_\Gamma^{\mathrm{el}}(z, [\![u]\!])\big)$$

and where $\Delta_\Gamma$ denotes the Laplace-Beltrami operator on $\Gamma$. This choice gives (78) with $\partial_z U_\Gamma^{\mathrm{el}}$ replaced by $\mathrm{D}_z\big(U_\Gamma^{\mathrm{el}} + G\big)$ and thus also results in a force balance alike (81)

$$0 \in \mathrm{D}_z\big(U_\Gamma^{\mathrm{el}}(z, [\![u]\!]) + G(\nabla z)\big) + \partial_{\dot z}\big(R_r(\dot z) + I_{(-\infty,0]}(\dot z)\big) \tag{86}$$

Moreover, we find for the fifth column in $\mathbb{L}_{E_\Gamma}$ that

$$-\tfrac{1}{2\partial_{\tau_\pm} E_\Gamma}\delta_z E_\Gamma \quad \text{is replaced by} \quad -\delta_z E_\Gamma\big[\tfrac{\square}{2\partial_{\tau_\pm} E_\Gamma}\big]\,, \tag{87}$$

where we have assumed homogeneous Neumann boundary conditions to hold along $\partial\Gamma$, here $\nabla z \cdot \mathrm{n}_\Gamma = 0$ on $\partial\Gamma$. This gives

$$-\delta_z E_\Gamma\big[\tfrac{\dot z}{2\partial_{\tau_\pm} E_\Gamma}\big] = -\Big(\zeta_z \cdot \tfrac{\dot z}{2\partial_{\tau_\pm} E_\Gamma} + \nabla_\Gamma z \cdot \nabla_\Gamma\big(\tfrac{\dot z}{2\partial_{\tau_\pm} E_\Gamma}\big)\Big) \tag{88}$$

to appear in (69d). To further process this expression we now assume that $\nabla z \cdot \nabla\big(\frac{\dot z}{2\partial_{\tau_\pm} E_\Gamma}\big)$ is formally equivalent to $-\Delta_\Gamma z\big(\frac{\dot z}{2\partial_{\tau_\pm} E_\Gamma}\big)$ thanks to the homogeneous Neumann boundary conditions. Hence, $-\delta_z E_\Gamma\big[\frac{\dot z}{2\partial_{\tau_\pm} E_\Gamma}\big]$ is formally replaced by $-\frac{1}{2\partial_{\tau_\pm} E_\Gamma}\mathrm{D}_z E_\Gamma \cdot \dot z$ in (69d). By repeating the arguments subsequent to (69d), we arrive at (72g) with $\delta_z E_\Gamma \cdot \dot z$ replaced by $\mathrm{D}_z E_\Gamma \cdot \dot z$. In this way we can again arrive at the interfacial coupling conditions (83) by exploiting the Fenchel equality, which now reads

$$\begin{aligned} &R_{\mathrm{D}}(q_{\Gamma\gamma};\dot z) + R^*_{\mathrm{D}}\Big(q_{\Gamma\gamma}; -\tfrac12(\tfrac{1}{\theta_+}+\tfrac{1}{\theta_-})\mathrm{D}_z\big(U^{\mathrm{el}}_\Gamma(z,[\![u]\!]) + G(\nabla z)\big)\Big) \\ &= \langle -\tfrac12(\tfrac{1}{\theta_+}+\tfrac{1}{\theta_-})\mathrm{D}_z\big(U^{\mathrm{el}}_\Gamma(z,[\![u]\!]) + G(\nabla z)\big), \dot z\rangle_\Gamma\,. \end{aligned}$$

**Remark 4.1.** We have shown at the example of delamination processes that the GENERIC structure of bulk-interface systems can be given in a weak sense based on thermodynamic functionals and geometric operators with bulk and interfacial contributions. The interfacial coupling conditions arise naturally from this weak form of GENERIC. The delamination models studied for their well-posedness, e.g., in the works [RR11, RT15] with $r = 1$ and in [BBR15a] with $r = 2$ are obtained from thermodynamic functionals as discussed in Sec.s 4.1 and 4.2. Hence above derivation confirms the GENERIC structure of these models. Yet, it has to be stressed that coupling conditions (72e)–(72h) and the reformulations made in Sec. 4.2 to arrive at (83) hold true on a formal level, only, since they require additional regularity of the terms involved, for example, for the term $\delta_z U^{\mathrm{el}}_\Gamma, \dot z$ appearing e.g. in (69d). However, for $r = 1$ this cannot be guaranteed, since $\dot z$ is a Radon measure, only, and to have good duality would thus require $\delta_z U^{\mathrm{el}}_\Gamma$ to be continuous, which clearly is not to be expected. To circumvent this problem [RR11, RT15] derive a weak formulation directly based on (83).

Finally, we remark that also sensitivity with respect to the fracture mode can be added to the model by decomposing the displacement jump $[\![u]\!] = [\![u]\!]\cdot \mathrm{n}_+ + [\![u]\!]\cdot \mathrm{t}$ into its normal and tangential components and by considering the $a(q)$ in (76) not only to depend on $\theta_\pm$ but also on a function $\alpha([\![u]\!]\cdot\mathrm{n}_+, [\![u]\!]\cdot\mathrm{t})$. In [RR13] the analysis of such a mode-sensitive adhesive contact model with thermal effects requires the use of higher order gradients of $\dot u$. ⋆

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