Internal Variables and Dynamic Degrees of Freedom

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Abstract

Dynamic degrees of freedom and internal variables are treated in a uniform way. The unification is achieved by means of the introduction of a dual internal variable. This duality provides the corresponding evolution equations depending on whether the Onsager–Casimir reciprocity relations are satisfied or not.

1. Introduction

Introduction of internal variables suggests taking into account the influence of an internal structure on the dynamic behavior of a material [1]. As long as evolution equations of internal variables are determined by general macroscopic principles, we can expect that the validity of the evolution equations is independent of particular microscopic models. It is important, therefore, to understand the universal aspects behind these evolution equations.

There are two basic methods to generate the evolution equations for internal variables. Both methods are based on fundamental principles.

The *first method* generates the evolution equations exploiting the entropy inequality. This approach uses exclusively thermodynamic principles, and the corresponding variables are called *internal variables of state* [2]. This framework has the advantage of operating with familiar thermodynamic concepts

(thermodynamic force, entropy); however, no inertial effects are considered. The thermodynamic theory of internal variables has a rich history (see the historical notes in [3]). A first more or less complete thermodynamic theory was suggested by Coleman and Gurtin [4], and a clear presentation of the general ideas was given by Muschik [5]. Internal variables were applied for several phenomena in different areas of physics, biology, and material sciences. A complete description of the thermodynamic theory with plenty of applications based on this concept of internal variables of state can be found in [6].

The *second method* generates the kinetic relations through a Hamiltonian variational principle and suggests that inertial effects are unavoidable. This approach has a mechanical flavor, and the corresponding variables are called *internal degrees of freedom*. Dissipation is added by dissipation potentials. This theoretical framework has the advantage of operating with familiar mechanical concepts (force, energy). The method was suggested by Maugin [7], and it also has a large number of applications [8,9]. A clear distinction between these two methods with a number of application areas is given by Maugin and Muschik [3, 10] and Maugin [2].

It is important to remark that the terminology of the field is not unique; more over, it is contradictory. For example, Verhás [6] calls his internal variables dynamic degrees of freedom following the suggestion of Kluitenberg (see, e.g., [11, 12]). Sometimes internal variables or internal degrees of freedom appear without thermodynamic foundation under different names. An important example can be found in nerve pulse dynamics, where the classical "phenomenological variables" of Hodgkin and Huxley [13] and the "recovery variables" of Nagumo, Arimoto, and Yoshizawa [14, 15] are internal variables from a thermodynamic point of view, as was shown in [16]. Another important example is damage mechanics (e.g., [17]), where the macroscopic damage variable is an internal variable from a thermodynamic point of view, and the thermodynamic framework can reveal several new properties of the theory [18, 19].

In this paper we follow the terminology of Maugin and Muschik [3] with some important extensions. We call internal variables of state those physical field quantities – beyond the classical ones – whose evolution is determined by thermodynamic - principles. We call internal degrees of freedom those physical quantities – beyond the classical ones – whose dynamics is determined by mechanical principles.

One of the questions concerning this doubled theoretical framework is related to common applications of variational principles and thermodynamics. Basic physical equations of thermodynamic origin do not have variational formulations, at least without any further ado [20]. That is well reflected

in the appearance of dissipation potentials as separate theoretical entities in variational models dealing with dissipation.

On the other hand, with pure thermodynamic methods – in the internal variables approach – inertial effects are not considered. Therefore, the coupling to simplest mechanical processes seemingly requires introducing some improvements, which are usually new principles of mechanical origin.

Therefore, one can have the impression that the doubling of the theoretical structure is a necessity, because the usage of both mechanical and thermodynamic principles cannot be avoided. This is the conceptual standpoint of the GENERIC approach (GEneral Non-equilibrium Equation of Reversible Irreversible Coupling) [21]. However, a doubled theoretical structure is not very convenient, because it doubles the number of physical assumptions restricting predictive capabilities of the theory.

In what follows, we propose a uniform approach based exclusively on thermodynamic principles. Our suggestion requires dual internal variables and a generalization of the usual postulates of non-equilibrium thermodynamics: we do not require the satisfaction of the Onsagerian reciprocity relations. With dual internal variables we are able to include inertial effects and to reproduce the evolution of dynamic degrees of freedom. It could be impossible with a single internal variable. This is the price we pay for the generalization. In other words, instead of the doubling of the theoretical structure, we suggest the doubling of the number of internal variables.

In the next section we give a short overview of the thermodynamic framework, then we summarize the theory of internal variables and internal degrees of freedom in Sections 3 and 4, respectively. The unified frame is developed in Section 5. Conclusions are given in the last section.

2.   Thermodynamics of continua

First, we recall the basic equations of the finite-strain thermoviscoelastic continua with internal variables. In this case, the state space of a material point $\mathbf{X}$ is spanned by the variables $(e, \mathbf{F}, \boldsymbol{\alpha})$, where e is the specific internal energy, $\mathbf{F}$ is the deformation gradient (direct-motion gradient) defined as $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}\big|_t$, and $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, ..., \alpha_n)$ are internal variables of state. Here $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ denotes the mapping from the reference configuration to an actual one.

The balance of linear momentum in an actual configuration reads (in the absence of body forces) [22]

$$\rho \dot{\mathbf{v}} - \nabla \cdot \mathbf{t} = \mathbf{0}, \tag{1}$$

where $\mathbf{v} = \frac{\partial \mathbf{x}}{\partial t} |_{\mathbf{X}}$ is the velocity field, the dot above the velocity denotes the substantial time derivative, and $\mathbf{t}$ is the Cauchy stress. The density ρ is not independent of the deformation gradient, because the density in the reference configuration is $\rho_0 = \rho \det \mathbf{F} = const$.

The balance of internal energy can be calculated as the difference between the conserved total energy and the kinetic energy and is given as (e.g., [6])

$$\rho \dot{e} + \nabla \cdot \mathbf{q} = \mathbf{t} : \dot{\mathbf{F}} \mathbf{F}^{-1}. \tag{2}$$

Here $\mathbf{q}$ is the heat flux and $\dot{\mathbf{F}} \mathbf{F}^{-1} = \nabla \mathbf{v}$. Then the entropy balance can be represented in the form [6, 22]

$$\rho \dot{s} + \nabla \cdot \mathbf{j} = \mathbf{q} \cdot \nabla \frac{1}{T} + \frac{1}{T} \left(\mathbf{t} - \mathbf{t}^{rev} \right) : \dot{\mathbf{F}} \mathbf{F}^{-1} - \frac{1}{T} \mathbf{A} \cdot \dot{\boldsymbol{\alpha}}. \tag{3}$$

Here we introduced the following traditional thermoelastic quantities (given by Gibbs's equation):

$$\frac{1}{T} = \frac{\partial s}{\partial e}, \quad \mathbf{t}^{rev} = \rho T \mathbf{F} \frac{\partial s}{\partial \mathbf{F}}, \tag{4}$$

$$\mathbf{A} = (A_1, A_2, ..., A_n) = \left(-\rho \frac{\partial s}{\partial \alpha_1}, -\rho \frac{\partial s}{\partial \alpha_2}, ..., -\rho \frac{\partial s}{\partial \alpha_n} \right). \tag{5}$$

The entropy s as a function of the state space variables $(e, \mathbf{F}, \boldsymbol{\alpha})$ is a concave function according to thermodynamic stability requirements.

It is important to emphasize that the entropy flux $\mathbf{j}$ in Eq. (3) is assumed to have its classical form

$$\mathbf{j}_{cl} = \frac{\mathbf{q}}{T}. \tag{6}$$

This is a severe assumption, and in the case of mixtures and weakly nonlocal extension of classical theories, the entropy flux deviates from this classical form as $\mathbf{j} = \frac{\mathbf{q}}{T} + \mathbf{J}$. This additional term was proposed first by Müller [23]. The particular form of the additional term $\mathbf{J}$ depends on the thermodynamic interactions and their level of nonlocality (e.g., in case of weakly nonlocal heat conduction, a family of its different forms is presented in [24]).

In what follows, we remind of the derivation of the evolution equations of internal variables from general principles. As the coupling to mechanical or thermal interactions could be involved and would blur the structure of equations, in the following we restrict ourselves to the case where the internal variables are completely decoupled from the mechanical and thermal interactions. Namely, this is the situation where the mechanical interaction is

reversible $\mathbf{t} = \mathbf{t}^{rev}$, the heat flux is zero $\mathbf{q} = \mathbf{0}$, $\rho = const.$, $\mathbf{v} = const.$, and there is a complete decoupling at the static level as well, that is

$$s(e, \mathbf{F}, \boldsymbol{\alpha}) = s_T(e) + s_M(\mathbf{F}) + s_A(\boldsymbol{\alpha}).$$

Let us remark that one can give very different conditions of decoupling, especially if other thermodynamic potentials are introduced, such as the Helmholtz free energy.

3. Internal variables of state

Let the basic thermodynamic state be spanned by n scalar internal variables $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, ..., \alpha_n)$. We want to determine their evolution according to thermodynamic principles.

3.1. Local state

Let us assume that the evolution equation of $\boldsymbol{\alpha}$ is given in a general form

$$\dot{\boldsymbol{\alpha}} = \mathbf{g}_\alpha, \tag{7}$$

where the dot denotes the material time derivative, which can be regarded as a partial one in our investigations.

The *local state hypothesis of Kestin* [25, 26] is introduced by the assumption that the entropy and the right-hand side of the evolution equation (7) are functions of $\boldsymbol{\alpha}$ and do not depend on the derivatives of the basic state. Furthermore, we assume that the entropy has a maximum in thermodynamic equilibrium, that is $\boldsymbol{\alpha} = \mathbf{0}$ at equilibrium. According to the Second Law, the entropy function is negative semidefinite and increasing along the processes determined by Eq. (7). Therefore, the entropy balance is given as

$$\dot{\rho}_s + \nabla \cdot \mathbf{J} = \sigma_s \geq 0. \tag{8}$$

Here $\rho_s = \rho s$ is the entropy density, $\mathbf{J} = \mathbf{j} - \frac{\mathbf{q}}{T}$ is the extra entropy flux, and $\nabla\cdot$ is the divergence operator.

Dissipation can be calculated according to Eq. (3),

$$T\sigma_s = -\mathbf{A} \cdot \mathbf{g}_\alpha = -\sum_{i=1}^{n} A_i g^i \geq 0, \tag{9}$$

where the thermodynamic affinity $\mathbf{A}$ conjugated to the internal variable $\boldsymbol{\alpha}$ is determined by Eq. (5) and $(\cdot)$ denotes a duality mapping onto the space of the internal variables as it is given by indexes.

3.2. Fluxes and forces

We may recognize a simple force-flux structure in Eq. (9) and identify $\mathbf{A}$ as a thermodynamic force and $\mathbf{g}_\alpha$ as a thermodynamic flux. A general solution of this inequality can be given in the form of so-called quasilinear *conductivity equations* [27, 28]:

$$\mathbf{g}_\alpha(\boldsymbol{\alpha}) = -\mathbf{L}(\mathbf{A}(\boldsymbol{\alpha}), \boldsymbol{\alpha})\mathbf{A}(\boldsymbol{\alpha}). \tag{10}$$

Substituting the latter into Eq. (7) results in a relaxation dynamics, because the conductivity matrix $\mathbf{L}$ is positive semidefinite, as a consequence of Eq. (9). We should make a distinction between this quasilinear case, where the conductivity matrix is a function of the forces and the state space ($\mathbf{L}(\mathbf{A}(\boldsymbol{\alpha}), \boldsymbol{\alpha})$), and the strictly linear case, where the conductivity matrix is constant ($\mathbf{L} = const$). The strictly linear theory is always an approximation that can be valid only in the vicinity of equilibrium.

The negative sign of the affinity is traditional and can be understood from the standard equilibrium formulation.

3.3. Dissipation potentials

General dissipation potentials were introduced by Onsager [29, 30] in the case of strictly linear conductivity equations. From the point of view of the general quasilinear conductivity equations (10), the existence of dissipation potentials is connected to the validity of the general Gyarmati–Li reciprocity relations [31, 32]. In our case, the Gyarmati–Li reciprocity relations in the so-called force representation [33] require that the derivative of the thermodynamic fluxes $\mathbf{g}_\alpha$ with respect to the thermodynamic forces (affinities $\mathbf{A}$), i.e., $\frac{\partial \mathbf{g}_\alpha}{\partial \mathbf{A}}(\mathbf{A}, \boldsymbol{\alpha})$, should be symmetric. This means that there exists a dissipation potential $D_A(\mathbf{A}, \boldsymbol{\alpha})$ with the property

$$\frac{\partial D_A}{\partial \mathbf{A}}(\mathbf{A}, \boldsymbol{\alpha}) = \mathbf{g}_\alpha(\mathbf{A}, \boldsymbol{\alpha}).$$

Formally, assuming a symmetric relation of the thermodynamic fluxes and forces, one can introduce the so-called flux representation [33] supposing that the thermodynamic forces are functions of the thermodynamic fluxes. In this case, the condition of the existence of the dissipation potential is connected to the validity of the related Gyarmati–Li reciprocity relations, that is, to the symmetry of the derivative $\frac{\partial \mathbf{G}_\alpha}{\partial A}(\mathbf{g}_\alpha, \boldsymbol{\alpha})$. As a result, we can get a flux-related dissipation potential D_g with the property

$$\frac{\partial D_g}{\partial \mathbf{g}_\alpha}(\mathbf{g}_\alpha, \boldsymbol{\alpha}) = \mathbf{A}(\mathbf{g}_\alpha, \boldsymbol{\alpha}).$$

In the strictly linear theory with a constant conductivity matrix $\mathbf{L}$, these two representations can be transformed into each other and both conditions coincide. Moreover, in this case the general Gyarmati–Li reciprocity relations become equivalent to the Onsagerian reciprocity relations. In the quasilinear case, they are not equivalent. It is also important to remark that the role of fluxes and forces is not completely interchangeable, because the fluxes are constitutive functions, and the forces are given functions of the constitutive state. Therefore, the validity of the flux representation is restricted mostly to the strictly linear theory.

3.4.   Weakly nonlocal internal variables

We now release the local state hypothesis and assume that the entropy is a function of both the internal variables and their gradients $(\boldsymbol{\alpha}, \nabla\boldsymbol{\alpha})$. Moreover, one can postulate ([3, 8]) that the extra entropy flux is

$$\mathbf{J} = -\left(\frac{\partial\rho_s}{\partial\nabla\boldsymbol{\alpha}}\right)\boldsymbol{g}_\alpha. \tag{11}$$

In this case, the entropy balance (8) together with the evolution equation (7) results in

$$\dot{\rho}_s(\boldsymbol{\alpha}, \nabla\boldsymbol{\alpha}) + \nabla\cdot\mathbf{J} =$$

$$= \frac{\partial\rho_s}{\partial\boldsymbol{\alpha}}\cdot\dot{\boldsymbol{\alpha}} + \frac{\partial\rho_s}{\partial\nabla\boldsymbol{\alpha}}\nabla\dot{\boldsymbol{\alpha}} - \nabla\cdot\left(\frac{\partial\rho_s}{\partial\nabla\boldsymbol{\alpha}}\boldsymbol{g}_\alpha\right) =$$

$$= \left(\frac{\partial\rho_s}{\partial\boldsymbol{\alpha}} - \nabla\cdot\frac{\partial\rho_s}{\partial\nabla\boldsymbol{\alpha}}\right)\cdot\boldsymbol{g}_a = -\mathrm{A}\cdot\boldsymbol{g}_\alpha \geq 0. \tag{12}$$

Now the thermodynamic flux is the same as in the local case, but the thermodynamic force has been changed to the new weakly nonlocal affinity $\mathrm{A} = -\frac{\partial\rho_s}{\partial\boldsymbol{\alpha}} + \nabla\cdot\frac{\partial\rho_s}{\partial\nabla\boldsymbol{\alpha}}$. Therefore, the evolution equation with quasilinear conductivity is

$$\dot{\boldsymbol{\alpha}} = \mathbf{L}\left(\frac{\partial\rho_s}{\partial\boldsymbol{\alpha}} - \nabla\cdot\frac{\partial\rho_s}{\partial\nabla\boldsymbol{\alpha}}\right). \tag{13}$$

It is remarkable that the right-hand side of the evolution equation becomes nonlocal as well.

The forces and the fluxes are compared in the following way:

Local force: $\frac{\partial \rho_s}{\partial \boldsymbol{\alpha}}(\boldsymbol{\alpha})$,   Nonlocal force: $\frac{\partial \rho_s}{\partial \boldsymbol{\alpha}}(\boldsymbol{\alpha}, \nabla \boldsymbol{\alpha}) - \nabla \cdot \frac{\partial \rho_s}{\partial \nabla \boldsymbol{\alpha}}(\boldsymbol{\alpha}, \nabla \boldsymbol{\alpha})$,

Local flux: $\mathbf{g}_a(\boldsymbol{\alpha})$,   Nonlocal flux: $\mathbf{g}_a(\boldsymbol{\alpha}, \nabla \boldsymbol{\alpha}, \nabla^2 \boldsymbol{\alpha})$.

Dissipation potentials can be generated as previously, but the previous local affinity **A** should be changed to the new weakly nonlocal affinity $\mathbb{A}$.

4. Internal degrees of freedom

Evolution equations of other microstructural variables – the *internal degrees of freedom* – are generated by mechanical principles. It is assumed that the dynamics of an internal degree of freedom $\boldsymbol{\alpha}$ is determined by a variational principle of Hamiltonian type with the Lagrangian $\mathcal{L}(\dot{\boldsymbol{\alpha}}, \boldsymbol{\alpha}, \nabla \boldsymbol{\alpha})$ and, therefore, it is governed by a field equation of the canonical form (e.g., [8]):

$$\frac{\delta \mathcal{L}}{\delta \boldsymbol{\alpha}} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\alpha}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{\alpha}}}\right) - \nabla \cdot \left(\frac{\partial \mathcal{L}}{\partial (\nabla \boldsymbol{\alpha})}\right) = \mathbf{f}_\alpha. \tag{14}$$

Here $\mathbf{f}_\alpha$ is the dissipative force and $\frac{\delta}{\delta \boldsymbol{\alpha}}$ is a functional derivative.

The Lagrangian $\mathcal{L}$ is usually divided into a kinetic and a potential part as follows:

$$\mathcal{L}(\dot{\boldsymbol{\alpha}}, \boldsymbol{\alpha}, \nabla \boldsymbol{\alpha}) = K(\dot{\boldsymbol{\alpha}}) - V(\boldsymbol{\alpha}, \nabla \boldsymbol{\alpha}). \tag{15}$$

Substituting this relation into Eq. (14), one can get the following particular form of the evolution equation for the internal degree of freedom $\boldsymbol{\alpha}$:

$$\frac{d^2 K}{d\dot{\boldsymbol{\alpha}}^2}\ddot{\boldsymbol{\alpha}} = -\frac{\partial V}{\partial \boldsymbol{\alpha}} + \nabla \cdot \frac{\partial V}{\partial \nabla \boldsymbol{\alpha}} - \mathbf{f}_\alpha, \tag{16}$$

where we have rearranged the terms to get an apparent Newtonian form.

One can consider higher order space derivatives and generate theories with higher order non-locality. On the other hand, one can apply the local state hypothesis, where the Lagrangian does not depend on the space derivatives, and the above equation simplifies. The natural boundary conditions for the internal degree of freedom are consequences of the variational formulation

$$\mathbf{T} = \left.\frac{\partial \mathcal{L}}{\partial \nabla \boldsymbol{\alpha}}\right|_{\partial V} \cdot \mathbf{n}, \tag{17}$$

where $\mathbf{n}$ is the normal of the boundary of the considered region ∂V at a given point and $\mathbf{T}$ is the surface "force" acting on the field $\boldsymbol{\alpha}$. The presence

and the nature of natural boundary conditions is sometimes connected to the observability and controllability of the internal degree of freedom [3].

Let us observe that the above mechanical description of the dynamics of the internal degree of freedom postulates a Hamiltonian variational principle and immediately generates a second-order differential equation in time (16). However, there is a natural way to get two first-order differential equations instead of a second-order one introducing the Hamiltonian through a suitable Legendre transformation. This transformation reveals some internal symmetries of the whole variational structure.

In fact, introducing a generalized momentum

$$\mathbf{p}_\alpha = \frac{\partial \mathcal{L}}{\partial \dot{\alpha}},$$

and a Hamiltonian H, defined by the partial Legendre transformation,

$$\mathbf{p}_\alpha \dot{\alpha} = \mathcal{L}(\dot{\alpha}, \alpha, \nabla\alpha) + H(\mathbf{p}_\alpha, \alpha, \nabla\alpha),$$

we arrive at the first Hamiltonian equation,

$$\dot{\alpha} = \frac{\partial H}{\partial \mathbf{p}_\alpha}. \tag{18}$$

On the other hand, the field equation (14) can be transformed, resulting in the second Hamiltonian equation,

$$\dot{\mathbf{p}}_\alpha = -\frac{\partial H}{\partial \boldsymbol{\alpha}} + \nabla \cdot \left(\frac{\partial H}{\partial (\nabla \boldsymbol{\alpha})} \right) - \mathbf{f}_\alpha. \tag{19}$$

Let us consider a particular form of the Hamiltonian equations in the case of the special Lagrangian given in Eq. (15). For simplicity, we also assume that the kinetic term K is quadratic, i.e., $K(\dot{\alpha}) = m\dot{\alpha}^2/2$, where $m = const$. In this case, the generalized momentum is $\mathbf{p}_\alpha = m\dot{\alpha}$, and one can get $\dot{\alpha}(\mathbf{p}_\alpha) = \mathbf{p}_\alpha/m$. The Hamiltonian follows as $H(\alpha, \mathbf{p}_\alpha) = \frac{\mathbf{p}_\alpha^2}{2m} + V(\boldsymbol{\alpha}, \nabla\boldsymbol{\alpha})$. Finally, the corresponding special Hamilton equations are

$$\dot{\alpha} = \frac{\mathbf{p}_\alpha}{m}, \tag{20}$$

$$\dot{\mathbf{p}}_\alpha = -\frac{\partial V}{\partial \boldsymbol{\alpha}} + \nabla \cdot \left(\frac{\partial V}{\partial (\nabla \boldsymbol{\alpha})} \right) - \mathbf{f}_\alpha. \tag{21}$$

4.1. Dissipation potentials

Some thermodynamic background can be added through the observation that the right-hand side of Eq. (14), the so-called *dissipative force* $\mathbf{f}_\alpha$, enters the entropy production because it generates dissipated power. The external mechanical power is included into the balance of total energy, then in the balance of internal energy (2), and, as a consequence, in the entropy balance (3), as well (another reasoning is based on the principle of virtual power [8, 34]). Finally, the entropy production can be written as

$$T\sigma_s = \mathbf{f}_\alpha \cdot \dot{\boldsymbol{\alpha}} \geq 0.$$

The whole thermodynamic formalism of the previous section can be repeated on the basis of the latter form of the entropy production, but now the thermodynamic fluxes are dissipative forces. However, here the thermodynamic formalism is added to the previous considerations of mechanical origin. For example, it is convenient to introduce dissipation potentials (with the above-mentioned conditions) D_f in the flux representation and put the dynamic equation (14) into the following form [3]:

$$\frac{\delta \mathcal{L}}{\delta \boldsymbol{\alpha}} = \frac{\partial D_f}{\partial \mathbf{f}_\alpha}.$$

5. Dual internal variables

As we have seen, evolution equations for internal variables of state and for internal degrees of freedom are completely different; cf. Eqs. (7) and (16). The same has been demonstrated recently on the example of continuum thermomechanics [2].

The question arises whether it is possible to construct a single way of derivation of evolution equations for both internal variables of state and internal degrees of freedom, or not?

A first guess may be that the internal variables of state are special cases of the internal degrees of freedom, because it looks very easy to get a first-order time-derivative equation from the second-order one. However, this is not the case. On the contrary, the structure of Hamiltonian differential equations (18) and (19) is very special. The essential part of the problem is that a second-order time-derivative equation can be generated by a Hamiltonian variational principle similar to the traditional variational principle in mechanics without any further ado, but a first-order time-derivative equation only in special constrained cases (gyroscopic degeneracy [35]). This is a strong mathematical restriction, and any attempt to circumvent the problem has the price of losing some parts of the nice Hamiltonian structure [20, 36].

Another important observation is that the dissipative part of the dynamics is generated by dissipation potentials also in the second, mechanical method. It is remarkable that the mechanical generation of evolution exploits thermodynamic methods.

In order to answer the formulated question, we introduce a dual internal variable and compare the arising evolution equations with the corresponding equations obtained in the previous sections.

Let us consider a thermodynamic system where the state space is spanned by two scalar internal variables, α, β. Then the evolution of these variables is determined by the following differential equations:

$$\dot{\alpha} = g_\alpha, \tag{22}$$

$$\dot{\beta} = g_\beta, \tag{23}$$

where the functions g_α and g_β of the right-hand side of the differential equations are constitutive functions and should be restricted by the Second Law of thermodynamics. The entropy inequality, the main ingredient of the Second Law, is the same as previously (Eq. (8)). Let the domain of the constitutive functions (our constitutive space) be spanned by the state space variables and by their first and second gradients. Therefore, our constitutive functions $g_\alpha, g_\beta, \mathbf{J}$, and ρ_s are given as functions of the variables $\alpha, \nabla\alpha, \nabla^2\alpha, \beta, \nabla\beta, \nabla^2\beta$. This is a weakly nonlocal constitutive space with second-order weak nonlocality in both variables.

5.1. Liu procedure

The Second Law restricts the form of the possible evolution equations (Eqs. (22)–(23)) and several exploitation methods of the Second Law can be implemented [37]. Here we apply the procedure of Liu [38].

The gradients of the constitutive functions g_α and g_β are constrained by the entropy inequality in the framework of a second-order constitutive state space for both of our variables as follows [39]:

$$\nabla\dot{\alpha} = \nabla g_\alpha(\alpha, \nabla\alpha, \nabla^2\alpha, \beta, \nabla\beta, \nabla^2\beta), \tag{24}$$

$$\nabla\dot{\beta} = \nabla g_\beta(\alpha, \nabla\alpha, \nabla^2\alpha, \beta, \nabla\beta, \nabla^2\beta). \tag{25}$$

Let us introduce the Lagrange–Farkas multipliers $\Lambda_\alpha, \Lambda_{\nabla\alpha}, \Lambda_\beta, \Lambda_{\nabla\beta}$ for Eqs. (22), (24), (23), and (25), respectively. Developing the partial derivatives of

the constitutive functions, we use the numbering of the variables of the constitutive state space spanned by $(\alpha, \nabla\alpha, \nabla^2\alpha, \beta, \nabla\beta, \nabla^2\beta)$ as a convenient and short notation, e.g., $\partial_3 \rho_s = \frac{\partial \rho_s}{\partial \nabla^2\alpha}$. Therefore, Eq. (8) can be written as follows:

$$
\begin{aligned}
&\dot{\rho}_s + \nabla \cdot \mathbf{J} - \Lambda_\alpha(\dot{\alpha} - g_\alpha) \\
&- \Lambda_{\nabla\alpha}(\nabla\dot{\alpha} - \nabla g_\alpha) - \Lambda_\beta(\dot{\beta} - g_\beta) - \Lambda_{\nabla\beta}(\nabla\dot{\beta} - \nabla g_\beta) = \\
&\partial_1\rho_s\dot{\alpha} + \partial_2\rho_s\nabla\dot{\alpha} + \partial_3\rho_s\nabla^2\dot{\alpha} + \partial_4\rho_s\dot{\beta} + \partial_5\rho_s\nabla\dot{\beta} + \partial_6\rho_s\nabla^2\dot{\beta} + \\
&\partial_1\mathbf{J}\cdot\nabla\alpha + \partial_2\mathbf{J}:\nabla^2\alpha + \partial_3\mathbf{J}\cdot:\nabla^3\alpha + \partial_4\mathbf{J}\cdot\nabla\beta + \partial_5\mathbf{J}:\nabla^2\beta + \\
&\partial_6\mathbf{J}\cdot:\nabla^3\beta - \Lambda_\alpha(\dot{\alpha} - g_\alpha) - \Lambda_{\nabla\alpha}(\nabla\dot{\alpha} - \partial_1 g_\alpha \cdot \nabla\alpha - \partial_2 g_\alpha : \\
&\nabla^2\alpha - \partial_3 g_\alpha \cdot : \nabla^3\alpha - \partial_4 g_\alpha \cdot \nabla\beta \partial_5 g_\alpha : \nabla^2\beta - \partial_6 g_\alpha \cdot : \nabla^3\beta) - \\
&\Lambda_\beta(\dot{\beta} - g_\beta) - \Lambda_{\nabla\beta}(\nabla\dot{\beta} - \partial_1 g_\beta \cdot \nabla\alpha - \partial_2 g_\beta : \nabla^2\alpha - \partial_3 g_\beta \cdot : \\
&\nabla^3\alpha - \partial_4 g_\beta \cdot \nabla\beta - \partial_5 g_\beta : \nabla^2\beta - \partial_6 g_\beta \cdot : \nabla^3\beta) \geq 0. \quad (26)
\end{aligned}
$$

Double and triple dots denote inner products of the corresponding tensors (scalars are formed). One can group together the coefficients by the derivatives of different orders:

$$
\begin{aligned}
&\dot{\alpha}\left(\partial_1\rho_s - \Lambda_\alpha\right) + \dot{\beta}\left(\partial_4\rho_s - \Lambda_\beta\right) + \\
&\nabla\dot{\alpha}\left(\partial_2\rho_s - \Lambda_{\nabla\alpha}\right) + \nabla\dot{\beta}\left(\partial_5\rho_s - \Lambda_{\nabla\beta}\right) + \\
&\nabla^2\dot{\alpha}\partial_3\rho_s + \nabla^2\dot{\beta}\partial_6\rho_s + \\
&\nabla^3\alpha\left(\partial_3\mathbf{J} + \Lambda_{\nabla\alpha}\partial_3 g_\alpha + \Lambda_{\nabla\beta}\partial_3 g_\beta\right) + \nabla^3\beta\left(\partial_6\mathbf{J} + \Lambda_{\nabla\alpha}\partial_6 g_\alpha + \Lambda_{\nabla\beta}\partial_6 g_\beta\right) + \\
&\nabla^2\alpha\left(\partial_2\mathbf{J} + \Lambda_{\nabla\alpha}\partial_2 g_\alpha + \Lambda_{\nabla\beta}\partial_2 g_\beta\right) + \nabla^2\beta\left(\partial_5\mathbf{J} + \Lambda_{\nabla\alpha}\partial_5 g_\alpha + \Lambda_{\nabla\beta}\partial_5 g_\beta\right) + \\
&\nabla\alpha\left(\partial_1\mathbf{J} + \Lambda_{\nabla\alpha}\partial_1 g_\alpha + \Lambda_{\nabla\beta}\partial_1 g_\beta\right) + \nabla\beta\left(\partial_4\mathbf{J} + \Lambda_{\nabla\alpha}\partial_4 g_\alpha + \Lambda_{\nabla\beta}\partial_4 g_\beta\right) + \\
&\Lambda_\alpha g_\alpha + \Lambda_\beta g_\beta \geq 0. \quad (27)
\end{aligned}
$$

We find the Liu equations as the coefficients of the derivatives that are not in the constitutive space:

$$
\dot{\alpha} : \partial_1\rho_s - \Lambda_\alpha = 0, \quad (28)
$$
$$
\dot{\beta} : \partial_4\rho_s - \Lambda_\beta = 0, \quad (29)
$$
$$
\nabla\dot{\alpha} : \partial_2\rho_s - \Lambda_{\nabla\alpha} = \mathbf{0}, \quad (30)
$$
$$
\nabla\dot{\beta} : \partial_5\rho_s - \Lambda_{\nabla\beta} = \mathbf{0}, \quad (31)
$$
$$
\nabla^2\dot{\alpha} : \partial_3\rho_s = \mathbf{0}, \quad (32)
$$
$$
\nabla^2\dot{\beta} : \partial_6\rho_s = \mathbf{0}, \quad (33)
$$
$$
\nabla^3\alpha : \partial_3\mathbf{J} + \Lambda_{\nabla\alpha}\partial_3 g_\alpha + \Lambda_{\nabla\beta}\partial_3 g_\beta = \mathbf{0}, \quad (34)
$$
$$
\nabla^3\beta : \partial_6\mathbf{J} + \Lambda_{\nabla\alpha}\partial_6 g_\alpha + \Lambda_{\nabla\beta}\partial_6 g_\beta = \mathbf{0}. \quad (35)
$$

The residual dissipation inequality follows from Eq. (27) by taking into account Eqs. (28)–(35):

$$(\partial_1 \mathbf{J} + \Lambda_{\nabla\alpha}\partial_1 g_\alpha + \Lambda_{\nabla\beta}\partial_1 g_\beta) \cdot \nabla\alpha + (\partial_4 \mathbf{J} + \Lambda_{\nabla\alpha}\partial_1 g_\alpha + \Lambda_{\nabla\beta}\partial_4 g_\beta) \cdot \nabla\beta +$$

$$(\partial_2 \mathbf{J} + \Lambda_{\nabla\alpha}\partial_2 g_\alpha + \Lambda_{\nabla\beta}\partial_2 g_\beta) : \nabla^2\alpha + (\partial_5 \mathbf{J} + \Lambda_{\nabla\alpha}\partial_5 g_\alpha + \Lambda_{\nabla\beta}\partial_5 g_\beta) : \nabla^2\beta +$$

$$\partial_1 \rho_s g_\alpha + \partial_4 \rho_s g_\beta \geq 0. \tag{36}$$

It is easy to see that higher than first-order derivatives of the constraints do not give additional restrictions, due to the simple structure of the evolution equations (22)–(23).

The solution of the Liu equations (28)–(33) leads to the entropy density, which is independent of the second gradients $\rho_s(\alpha, \nabla\alpha, \nabla^2\alpha, \beta, \nabla\beta, \nabla^2\beta) = \hat{\rho}_s(\alpha, \nabla\alpha, \beta, \nabla\beta)$, and its partial derivatives are the Lagrange–Farkas multipliers:

$$\Lambda_\alpha = \partial_1 \rho_s = \frac{\partial \hat{\rho}_s}{\partial \alpha}, \quad \Lambda_{\nabla\alpha} = \partial_2 \rho_s = \frac{\partial \hat{\rho}_s}{\partial \nabla\alpha}, \quad \Lambda_\beta = \partial_4 \rho_s = \frac{\partial \hat{\rho}_s}{\partial \beta},$$

$$\Lambda_{\nabla\beta} = \partial_5 \rho_s = \frac{\partial \hat{\rho}_s}{\partial \nabla\beta}.$$

Substituting the Lagrange–Farkas multipliers into Eqs. (34) and (35), one can solve them and get the entropy flux:

$$\mathbf{J}(\alpha, \nabla\alpha, \nabla^2\alpha, \beta, \nabla\beta, \nabla^2\beta) = -\partial_2 \rho_s g_\alpha - \partial_5 \rho_s g_\beta + \mathbf{j}_0 =$$

$$-\frac{\partial \hat{\rho}_s}{\partial \nabla\alpha} g_\alpha - -\frac{\partial \hat{\rho}_s}{\partial \nabla\beta} g_\beta + \mathbf{j}_0. \tag{37}$$

Here the additional entropy flux term $\mathbf{j}_0$ is a function only of the variables $(\alpha, \nabla\alpha, \beta, \nabla\beta)$, as well as ρ_s. Substituting this expression into the dissipation inequality, we get finally:

$$\sigma_s = (\partial_1 \rho_s - \nabla \cdot \partial_2 \rho_s) g_\alpha + (\partial_4 \rho_s - \nabla \cdot \partial_5 \rho_s) g_\beta + \nabla \cdot \mathbf{j}_0 =$$

$$\left(\frac{\partial \hat{\rho}_s}{\partial \alpha} - \nabla \cdot \frac{\partial \hat{\rho}_s}{\partial \nabla\alpha} \right) g_\alpha + \left(\frac{\partial \hat{\rho}_s}{\partial \beta} - \nabla \cdot \frac{\partial \hat{\rho}_s}{\partial \nabla\beta} \right) g_\beta + \nabla \cdot \mathbf{j}_0 \geq 0. \tag{38}$$

Let us remember that $\hat{\rho}_s$ is independent of the second gradients of the variables, therefore there are no higher derivatives in Eq. (38). Let us assume now that $\mathbf{j}_0 = \mathbf{0}$. This is an assumption that we regularly consider in classical irreversible thermodynamics excluding the appearance of current multipliers and terms similar to those that appeared in the Guyer–Krumhansl equation [28, 40]. We may recognize an Onsagerian force-flux system, where the

thermodynamic fluxes and forces are

$$\alpha\text{-force:} \quad A = -\frac{\partial \rho_s}{\partial \alpha} + \nabla \cdot \frac{\partial \rho_s}{\partial \nabla \alpha}, \qquad \alpha\text{-flux:} \quad g_\alpha,$$

$$\beta\text{-force:} \quad B = -\frac{\partial \rho_s}{\partial \beta} + \nabla \cdot \frac{\partial \rho_s}{\partial \nabla \beta}, \qquad \beta\text{-flux:} \quad g_\beta.$$

Here we introduce a shortened notation A and B for the thermodynamic forces, preserving the sign conventions of the previous sections.

5.2. Evolution equations

The solution of the inequality (38) can be represented as

$$\begin{pmatrix} g_\alpha \\ g_\beta \end{pmatrix} = -\mathbf{L} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} l_1 & l_{12} \\ l_{21} & l_2 \end{pmatrix} \begin{pmatrix} -A \\ -B \end{pmatrix}. \tag{39}$$

This corresponds to the inequality (38) if the Onsagerian coefficients l_1, l_2, l_{12}, l_{21} are functions of the thermodynamic forces A and B and the state variables $(\alpha, \nabla\alpha, \beta, \nabla\beta)$. Signs of the coefficients should be further restricted by the requirement of nonnegative entropy production.

In what follows, we split the conductivity matrix into a symmetric and an antisymmetric part, introducing k and l instead of l_{12} and l_{21} by $l_{12} = l - k$ and $l_{12} = l + k$:

$$\dot{\alpha} = g_\alpha = kB - l_1 A - lB, \tag{40}$$

$$\dot{\beta} = g_\beta = -kA - lA - l_2 B. \tag{41}$$

The nonnegativity of the entropy production (38) results in the positive semi-definiteness of the symmetric part of the conductivity matrix $\mathbf{L}$. Therefore, the following inequalities are valid for the coefficients:

$$l_1 \geq 0, \quad l_2 \geq 0, \quad l_1 l_2 - l^2 \geq 0. \tag{42}$$

5.3. Remark on dissipation potentials

We may introduce dissipation potentials for the dissipative part of the equations, if the condition of their existence is satisfied. However, in the considered case there is no need of this assumption, because here it is clear what belongs to the dissipative part and what belongs to the nondissipative part of the the

evolution equations. The terms with the symmetric conductivity contribute to the entropy production and the terms from the skew symmetric part do not. On the other hand, there is no need of potential construction, as we are not looking for a variational formulation. Moreover, the symmetry relations are not sufficient for the existence of dissipation potentials in general, as we have emphasized previously. In the case of constant coefficients (strict linearity), the dissipation potentials always exist for the dissipative (symmetric) part.

5.4. Remark on the reciprocity relations

The reciprocity relations are the main results of the great idea of Lars Onsager connecting fluctuation theory to macroscopic thermodynamics [29, 30, 41–43]. As it was written by Onsager himself on the validity of his result: "The restriction was stated: on a kinetic model, the thermodynamic variables must be algebraic sums of (a large number of) molecular variables, and must be *even* functions of those molecular variables which are odd functions of time (like molecular velocities)" [42]. The Casimir reciprocity relations are based on microscopic fluctuations, too [43]. We do not have such a microscopic background for most of internal variables. E.g., in the case of damage we think that the internal variables are reflecting a structural disorder on a mesoscopic scale. The relation between thermodynamic variables and the microscopic structure is hopelessly complicated. On the other hand, the Onsagerian reciprocity is based on time reversal properties of corresponding physical quantities either at the macro or at the micro level. Looking for the form of evolution equations without a microscopic model, we do not have any information on the time reversal properties of our physical quantities neither at the micro- nor at the macroscopic level. Therefore, we can conclude that lacking the conditions of the Onsagerian or Casimirian reciprocity gives no reason to assume their validity in the internal variable theory.

Let us observe the correspondence of evolution equations for internal variables with the reciprocity relations by means of a few simple examples.

5.5. Example 1: Internal variables of state

Let us consider materials with zero antisymmetric part of the conductivity matrix $\mathbf{L}$ ($l = 0$, $k = 0$). It is clear that the Onsagerian reciprocity relations are satisfied, and we return to the classical situation with fully uncoupled

internal variables:

$$\dot{\alpha} = g_\alpha = -l_1 A, \tag{43}$$

$$\dot{\beta} = g_\beta = -l_2 B. \tag{44}$$

In this case, the evolution equations for dual internal variables α and β are the same as in the case of single internal variable of state (Eq. (13)).

5.6.   Example 2: Internal degrees of freedom

We now assume that all conductivity coefficients are constant, and their values are $l_1 = l = 0$, $k = 1$. This means that $l_{12} = -l_{21}$, i.e., the Casimirian reciprocity relations are satisfied.

For simplicity, we decompose the entropy density into two parts, which are dependent on different internal variables:

$$\rho_s(\alpha, \nabla\alpha, \beta, \nabla\beta) = -K(\beta) - W(\alpha, \nabla\alpha). \tag{45}$$

The negative signs are introduced taking into account the concavity of the entropy. Then the thermodynamic forces are represented as

$$A = \frac{\partial W}{\partial \alpha} - \nabla \cdot \frac{\partial W}{\partial \nabla\alpha}, \qquad B = \frac{dK}{d\beta} = K'(\beta),$$

and Eqs. (40) and (41) are simplified to

$$\dot{\alpha} = g_\alpha = B = K'(\beta) \tag{46}$$

$$\dot{\beta} = g_\beta = -A + l_2 B = -\frac{\partial W}{\partial \alpha} + \nabla \cdot \frac{\partial W}{\partial \nabla\alpha} - l_2 K'(\beta). \tag{47}$$

One may recognize that the obtained system of equation corresponds exactly to what was introduced in the case of dynamic degrees of freedom after transforming the equation of motion into a Hamiltonian form, Eqs. (18) and (19).

The transformation into a Lagrangian form is trivial if K is quadratic: $K(\beta) = \frac{\beta^2}{2m}$, where m is a constant. Then we get exactly Eqs. (20) and (21) and the whole system corresponds to Eq. (5.14) in [3] with the Lagrangian

$$\mathcal{L}(\dot{\alpha}, \alpha, \nabla\alpha) = m\frac{\dot{\alpha}^2}{2} - W(\alpha, \nabla\alpha) \quad \text{and} \quad D(\alpha, \dot{\alpha}) = \frac{ml_2}{2}\dot{\alpha}^2.$$

Moreover, the entropy flux density (37) in the case of our special conditions can be written as

$$\mathbf{J} = -\frac{\partial \rho_s}{\partial \nabla \alpha} K'(\beta) + \mathbf{j}_0, \tag{48}$$

and one can infer that natural boundary conditions of the variational principle (17) correspond to the condition of vanishing entropy flow at the boundary, i.e., $\mathbf{j}_0 = \mathbf{0}$.

Therefore, the variational structure of internal degrees of freedom is recovered in the pure thermodynamic framework. The thermodynamic structure resulted in several sign restrictions of the coefficients, and the form of the entropy flux is also recovered. The natural boundary conditions correspond to a vanishing extra entropy flux.

5.7. Example 3: Diffusive internal variables

Now we give an additional example to see clearly the reduction of evolution equations of internal degrees of freedom to evolution equations for internal variables and the extension of the latter to the previous one.

We keep the values of conductivity coefficients (i.e., $l_1 = l = 0$, $k = 1$) but assume that both K and W are quadratic functions:

$$K(\beta) = \frac{b}{2}\beta^2, \quad W(\alpha, \nabla \alpha) = \frac{a}{2}(\nabla \alpha)^2,$$

where a and b are positive constants according to the concavity requirement.

In this case, the evolution equations (46), (47) reduce to

$$\dot{\alpha} = g_\alpha = B = K'(\beta) = b\beta, \tag{49}$$

$$\dot{\beta} = g_\beta = -\frac{\partial W}{\partial \alpha} + \nabla \cdot \frac{\partial W}{\partial \nabla \alpha} - l_2 K'(\beta) = a\Delta\alpha - l_2 b\beta. \tag{50}$$

Substituting β from Eq. (49) into Eq. (50), we have

$$\frac{1}{ab}\ddot{\alpha} + \frac{l_2}{a}\dot{\alpha} = \Delta\alpha, \tag{51}$$

which is a Cattaneo–Vernotte-type hyperbolic equation (telegraph equation) for the internal variable α. This can be considered as an extension of a diffusion equation by an inertial term or as an extension of a damped Newtonian equation (without forces) by a diffusion term.

6.   Conclusions

In the framework of the thermodynamic theory with dual weakly nonlocal internal variables presented in this paper, we are able to recover the evolution equations for internal degrees of freedom.

We have seen that the form of evolution equations depends on the mutual interrelations between the two internal variables. In the special case of internal degrees of freedom, the evolution of one variable is driven by the second one, and vice versa. This can be viewed as a duality between the two internal variables. In the case of pure internal variables of state, this duality is replaced by self-driven evolution for each internal variable. The general case includes all intermediate situations.

It is generally accepted that internal variables are "measurable but not controllable" (see, e.g., [25]). Controllability can be achieved by boundary conditions or fields directly acting on the physical quantities. We have seen how natural boundary conditions arise considering nonlocality of the interactions through weakly nonlocal constitutive state spaces.

As we wanted to focus on generic inertial effects, our treatment is simplified from several points of view. Vectorial and tensorial internal variables were not considered and the couplings to traditional continuum fields result in degeneracies and more complicated situations than in our simple examples.

Let us mention here the related pioneering works of Verhás, where skew symmetric conductivity equations appear in different inspiring contexts [44, 45].

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