

Irreversible thermodynamics from the point of view of internal variable theory (a Lagrangian formulation)

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A LAGRANGIAN density function is introduced. Variational principles are derived. The adjoint system is introduced and its importance for inverse problems is discussed.

Zaproponowano funkcję gęstości Lagrange'a. Wyprowadzono zasady wariacyjne. Zdefiniowano układ sprzężony i przedyskutowano jego znaczenie dla problemu odwrotnego.

Введена функция плотности Лагранжа. Введены вариационные принципы. Определенная система и обсуждено ее значение для обратной задачи.

General discussion

IN A SERIES of papers VALANIS [14, 15, 16], COLEMAN and GURTIN [4, 11], RICE [13], LUBLINER [9] and others have considered the averaging effects of the internal structure on the constitutive properties of a deforming solid by introducing internal variables. These represent, roughly speaking, the averages, of some molecular or atomic displacements. In this paper the internal variables will be denoted by q_α , $\alpha = 1, 2, \dots, n$. These variables are adjoined to observable thermodynamic variables such as temperature (or entropy) and strain.

Despite very serious objections of both physical and mathematical nature (see Appendix 2), we are going to adhere to tradition by offering a pointwise definition of a thermodynamic process, specifying in a region $\mathcal{B} \subset \mathcal{R}^3$ the functions θ , \mathbf{q} , defined (a.e) pointwise in \mathcal{B} . See modern monographs such as TRUESDELL's work [21] or COLEMAN, MARKOVITZ and NOLL [4] for rigorous mathematical definitions following this point of view. This is done purely for the sake of simplicity. Thus we regard, for example, the temperature θ as a positive function defined (a.e.) at each point \mathcal{B} , rather than a set valued function whose domain are subsets of \mathcal{B} , of positive Borel measure.

It is clear that a microsystem can not be regarded as arbitrarily small, or infinitesimal, if the concepts of average physical quantities such as energy density, stress, entropy density, are to be physically significant in a physical medium which is made of particles. This is so since at an atomic level these quantities are either undefined or at best badly discontinuous. In the case of polymeric materials, regarding them as dissipative thermodynamic systems, Valanis identified the internal variables as actual displacements along a typical very large molecule. Hence, in the study of polymers \mathbf{q}_α could be identified with average displacements and corresponding generalized forces could be identified with the energy gradient $\partial\psi/\partial q_\alpha$.

Here, q_α , $\alpha = 1, 2, \dots, n$, were discrete variables (see [19] for details). In this paper we shall pursue this line of approach, for convenience retaining pointwise definitions, but also retaining a strong mental reservation about all physical properties defined pointwise in \mathcal{B} .

We also follow a procedure which was originally introduced by Duhem and Hadamard by defining (for each point of \mathcal{B}) the specific internal energy density function ε . In the case considered here ε is assumed to depend on the temperature (or entropy), on the deformation, and on the internal variables q_α . Specifically:

$$(1) \quad \varepsilon = \varepsilon(\theta, \mathbf{C}, q_\alpha),$$

where θ is the temperature, and \mathbf{C} is the right Cauchy-Green deformation tensor. We also introduce the Helmholtz free energy density function pointwise defined:

$$(2) \quad \psi = \varepsilon - \eta\theta,$$

where η is the entropy density function.

1. Internal variables—the discrete case

The studies made in [19] regarding polymers have been generalized to other materials, the internal variables being still identified with statistical averages of displacements of material points at a microsystem level. It is an easy mental transition to associate such statistical averages of generalized displacements with the internal variables q_α , and to introduce the corresponding generalized forces:

$$-Q_\alpha = \frac{\partial \psi}{\partial q_\alpha},$$

generalized velocities:

$$(1.1) \quad \dot{q}_\alpha,$$

generalized viscous friction:

$$(1.2) \quad \sum_{j=1}^n b_{\alpha j} \dot{q}_j,$$

and generalized inertia $m_\alpha \ddot{q}_\alpha$, so that in the absence of internal forces one obtains the internal equations

$$(1.3) \quad \frac{\partial \psi}{\partial q_\alpha} + \sum_{j=1}^n b_{\alpha j} \dot{q}_j + m_\alpha \ddot{q}_\alpha = 0 \quad (\alpha \text{ not summed}).$$

In [16] VALANIS has observed that the Clausius-Duhem inequality is violated if ψ is identified with the Helmholtz free energy $\bar{\psi}$. However, this defect is rectified if an appropriate kinetic energy term is added to $\bar{\psi}$, and the free energy density ψ becomes

$$(1.4) \quad \psi = \bar{\psi} + \frac{1}{2} \sum_{\alpha=1}^n m_\alpha (\dot{q}_\alpha)^2.$$

If γ denotes the irreversible entropy (i.e. $\dot{\gamma} = \dot{\eta} + \frac{h_\alpha}{\theta}$, h_α denoting the heat flux vector)

$$(1.5) \quad \theta \dot{\gamma} = - \sum_{\alpha=1}^n Q_\alpha \dot{q}_\alpha > 0; \quad (\text{see [16]}).$$

The analogy between the dissipation term $\theta \dot{\gamma}$ and $Q_\alpha \dot{q}_\alpha$ suggest that the temperature could be regarded as a generalized force if the entropy is considered to be the $(n+1)$ generalized displacement provided the distributed internal variables q_α are introduced. A philosophic discussion of mechanical interpretation of entropy and temperature will be given later in a future paper. For the time being we shall simply introduce a formal notation in which q_α , $\alpha = 1, 2, \dots, n, n+1$, are the internal variables and we identify entropy as q_{n+1} .

In the discrete case the equations of motion (1.3) are easily derived as Lagrange equations

$$(1.6) \quad \frac{\partial \psi}{\partial q_\alpha} + \frac{d}{dt} \left(\frac{\partial \psi}{\partial \dot{q}_\alpha} \right) = - \sum_{j=1}^n b_{\alpha j} \dot{q}_j = -f_\alpha,$$

where ψ — the Largangian density function — is analogous to the Lagrangian density function of classical mechanics, expressing the difference of kinetic and potential energy densities while f_α are internal friction forces.

Thus

$$(1.7) \quad \mathcal{L} = \sum_{i=1}^n \frac{1}{2} m_i (\dot{q}_i)^2 - \bar{\psi},$$

where $\bar{\psi}$ is the Helholtz free energy density function. Before proceeding from the discrete case to the case when q_α are distributed variables, we would like to redefine the terms of say Eq. (1.6) for the case when ψ is a functional depending on the (pointwise defined a.e. in \mathcal{B}) functions \mathbf{q} , $\dot{\mathbf{q}}$. The classical derivatives will be replaced by Fréchet (or Gateaux) derivatives (see Appendix 1) without major changes in the arguments.

For the sake of clarifying the subsequent discussion we shall first introduce a simple mechanical example.

2. A simple example

To illustrate the basic concepts and corresponding extension of a classical treatment we consider a mechanical system which is a one-dimensional elastic body (a rod) subjected to certain time dependent compressive or tensile forces (stresses) at the boundary. For simplicity's sake the boundary is assumed to consist of a single point with either the rod extending to $-\infty$, or else being rigidly held at some point to which we have no access.

We are capable of observing only the state variables (displacement, stress) at the boundary point B , and do not have any means of observing the state variables at interior points.

We identify the deformation function $q(x, t)$ which assigns to the point occupied at time t , the point of the rod which was at the coordinate x at the time t_0 . We denote $\xi = q(x, t_0)$. The subscript t_0 can be omitted, and we assume that the material density, cross-sectional area and the length of the rod are approximately constant. See later the discussion for a rigorous explanation of "approximately constant".

We have no physical means of observing the values of $q(x, t)$ except at the boundary point $x = 1$.

However, the kinetic energy T and potential energy V are easily computed for a given function $q(x, t)$

$$T(t) = \frac{\rho}{2} \int_0^1 (\dot{q}(x, t))^2 dx,$$

$$V(t) = \frac{A}{2} \int_0^1 E(x) \left(\frac{\partial q(x, t)}{\partial x} \right)^2 dx.$$

We refer to $q(x, t)$ as an internal variable. $\dot{q} = \frac{\partial q(x, t)}{\partial t}$ can be called the internal velocity, $\frac{\partial q(x, t)}{\partial x}$ the internal deformation gradient. Note that $C = q(1, t)$ is the Cauchy-Green tensor which is observable.

So far no dissipation has been introduced and $q(x, t)$ must satisfy the differential equations arising from the Euler-Lagrange principle of stationary behaviour of the action integral

$$\delta \int_{t_0}^t (T - V) dt = 0.$$

In this case we obtain a classical form of the wave equation in one space dimension for $q(x, t)$.

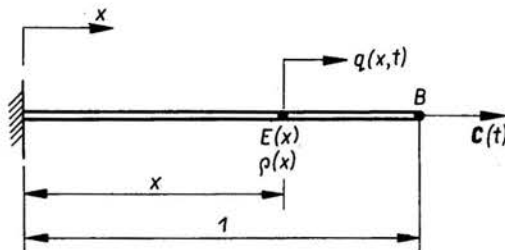


FIG. 1.

Let us complicate slightly the example shown on Fig. 1 by introducing viscous damping and some forces transmitted at a distance from one part of the rod to another.

We can think of enclosing the rod in a vessel with a viscous fluid, and attaching some linear springs to various points of the rod. (Let us label these points x, x' .)

Strictly, there is of course no such thing as an instant transmission of forces at a distance, since at least the velocity of light presents a definite barrier to instant “communications” between different parts of the material. This is not, however, a serious objection to the physical usefulness of our mathematical model in cases when the speed of prop-

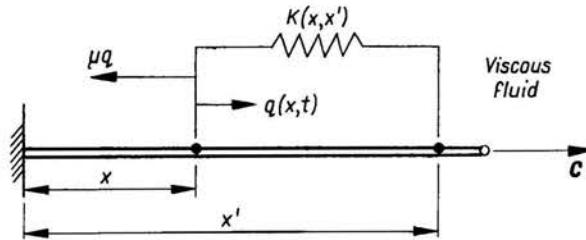


FIG. 2.

agation of information about the state of the material is large compared to the rates of processes in the material.

The kinetic energy is still of the form

$$T(t) = \frac{1}{2} \int_0^1 \frac{p(x) (\dot{q})^2}{2} dx.$$

The Helmholtz free energy (potential energy) becomes

$$\Psi(t) = \frac{A}{2} \int_0^1 \int_0^1 K(x, \zeta) \frac{\partial q(x, t)}{\partial x} \frac{\partial q(\zeta, t)}{\partial \zeta} \partial x d\zeta,$$

where \$K(x, \zeta)\$ is positive \$L_2(0, 1)\$ function.

The kernel \$K(x, \zeta)\$ being square integrable, i.e.

$$\int_0^1 \int_0^1 (K(x, \zeta))^2 dx d\zeta < \infty$$

implies that the transformation \$T\$ defined by

$$\phi(x) = \int_0^1 f(\zeta) K(x, \zeta) = Tf(x)$$

is of the Hilbert-Schmidt type, i.e. the operator \$T\$ is a Hilbert-Schmidt operator, hence it is compact.

If \$K(x, \zeta) = K(\zeta, x)\$, which is reasonable in our model where \$E(x)\$ is modified by attaching linear springs (after all it is Betti’s reciprocity principle), then the spectrum of \$T\$ lies on the positive part of the real line, and is discrete, with zero as the only possible accumulation point of the spectrum.

We can introduce a space \$\mathcal{H}\$ with the following product for any \$u, v \in \mathcal{H}: \langle u, v \rangle = \tilde{T}(u, v) + \tilde{\psi}(u, v) + \tilde{D}(u, v)\$, where the products \$\tilde{T}, \tilde{\psi}, \tilde{D}\$ are defined as

$$\tilde{T}(u, v) = \frac{\rho}{2} \int_0^1 \frac{\partial u(t, x)}{\partial t} \frac{\partial v(t, x)}{\partial t} dx,$$

$$\tilde{\Psi}(u, v) = \frac{A}{4} \int_0^1 K(x, \zeta) \left\{ \frac{\partial u(t, x)}{\partial x} \frac{\partial v(t, \zeta)}{\partial \zeta} + \frac{\partial u(t, \zeta)}{\partial \zeta} \frac{\partial v(t, x)}{\partial x} \right\} dx d\zeta,$$

$$\tilde{D}(u, v) = \frac{1}{2} \int_0^1 \mu(x) \frac{\partial u(t, x)}{\partial t} v(t, x) dx.$$

When $\mu = 0$ (hence $\tilde{D}(u, v) = 0$), \mathcal{H} can be identified with the Sobolev space $W_2^{1,1}$. (For definitions, see [10] and Appendix 2.)

Observe that $\langle u, u \rangle > 0$, if $u \neq 0$, and the triangular inequality has to be satisfied by physical arguments. Therefore \mathcal{H} is a metric space, $d(u, v) = \langle u-v, u-v \rangle$ defining the distance.

$$\tilde{\mathcal{L}}(u, v) = \tilde{T}(u, v) - (\tilde{\Psi}(u, v) + \tilde{D}(u, v))$$

will be called the Lagrangian product of u and v .

If the kernel $K(x, \zeta)$ is symmetric, the expression for the Helmholtz free energy product can be simplified:

$$\tilde{\Psi}(u, v) = \frac{A}{2} \int_0^1 \int_0^1 K(x, \zeta) \frac{\partial u(t, x)}{\partial x} \frac{\partial v(t, \zeta)}{\partial \zeta} dx d\zeta.$$

Obviously the value of $\tilde{\Psi}(u, v)$ is invariant under the interchange of the variables x and ζ .

Fréchet differentiation with respect to v now yields exactly the equations of motion of the rod. This simple example was specifically produced to demonstrate a number of concepts. The internal variable q (identified with $u(t, x)$ in a subsequent discussion) was shown to obey a partial differential equation of the wave type

$$\frac{\partial q^2}{\partial x^2} - \frac{1}{C^2} \frac{\partial^2 q}{\partial t^2} = f(x, t) \quad \text{where} \quad f \text{ is } \mu(x) \frac{\partial u}{\partial t}$$

derived from the Euler-Lagrange necessary condition for an extremum of the Lagrangian functional $\tilde{\mathcal{L}}(u, v) = \tilde{T} - (\tilde{\Psi} + \tilde{D})$, by setting the Fréchet derivative $\tilde{\mathcal{L}}_v = 0$. (See Appendix 1.)

So far the discussion was limited to a simple example of mechanics, with no heat flux, and no changes considered in the thermodynamic variable θ, η .

It is the purpose of the next section of this paper to extend the concepts illustrated in Sect. 2 to a description of an irreversible process allowing us to average the microscopic phenomena, and to introduce corresponding variables in the language of classical continuum mechanics.

3. The notion of internal generalized forces and of internal generalized momenta

The existence almost everywhere of the Helmholtz free energy density function $\bar{\psi}$ is postulated.

The total free energy density function is defined by

$$(3.1) \quad \psi = \bar{\psi} + \frac{1}{2} \sum_i \varrho(\dot{q}_i)^2,$$

where q_i are distributed internal variables.

Following VALANIS [16] we define the internal inertia to be $-\varrho\ddot{q}_i$, and we can define the internal (generalized) momentum

$$(3.2) \quad p_i = \frac{\partial \hat{\psi}}{\partial \dot{q}_i} \quad (\text{or } \hat{\psi}_{\dot{q}_i} \text{ in a simplified notation})$$

where $\partial/\partial \dot{q}_i$ or the subscript \dot{q}_i denotes the Fréchet derivative of the functional $\hat{\psi}$ with respect to the vector \dot{q}_i , where tacitly it is assumed that $\hat{\psi}$ is Fréchet differentiable.

Q_i will denote the generalized (distributed) force corresponding to the internal displacement q_i

$$(3.3) \quad -Q_i = \frac{\partial \hat{\psi}}{\partial q_i}.$$

We observe that the rate of work performed by the generalized force Q_i is given by

$$(3.4) \quad W_i = \langle Q_i, \dot{q}_i \rangle = - \left\langle \frac{\partial \hat{\psi}}{\partial q_i}, \dot{q}_i \right\rangle.$$

If pointwise description is used, then the density of W_i at a point is defined by $Q_i \dot{q}_i$. The stress-strain relationship is obtained simply by setting $x = 1$.

At this point we shall make the following observation. Carefully distinguishing the temperature from the internal (displacement) variables, we obtain identical mathematical formulas for each q_i and θ .

If the Helmholtz free energy ψ depends on temperature, and the existence of entropy is either postulated or proved, following some axioms (see [16]), then $\eta = -\frac{\partial \psi}{\partial \theta}$ can be regarded as another generalized force associated with the generalized displacement θ .

The total rate of work performed by the generalized forces is

$$(3.5) \quad W = -\theta \dot{\eta} + \sum_{i=1}^n -\frac{\partial \hat{\psi}}{\partial q_i} \dot{q}_i = - \sum_{i=1}^{n+1} \frac{\partial \hat{\psi}}{\partial q_i} \dot{q}_i,$$

where $q_{n+1} = \theta$, and

$$\eta = -\frac{\partial \hat{\psi}}{\partial q_{n+1}} = Q_{n+1}.$$

As before all derivatives are regarded as Fréchet derivatives.

We recognize $\hat{W} = -h_x$ as the rate of heat flux which balances the work performed by the internal forces Q_i , $i = 1, 2, \dots, n+1$.

Equation (3.5) is in fact an entropy balance statement. The equations (3.1)–(3.5) are understood to be defined pointwise almost everywhere in the distributed parameter case. A generalization to weak solution of Eqs. (3.1)–(3.5) is fairly trivial, involving the appli-

cation of the definition, i.e. for all ϕ in a suitable class Φ of test functions it is true that, for example,

$$(3.6) \quad \langle -h_{\alpha}^{\alpha}, \phi \rangle = \langle \theta, (\eta\phi)' \rangle - \sum_i \left\langle q_i, \left(\frac{\partial \psi}{\partial q_i} \phi \right)' \right\rangle \quad \text{etc.,}$$

where $\langle, \rangle_{\Omega}$ denotes in this case the usual $L_2(\Omega)$ product, Ω being the region of \mathcal{R}^3 occupied by the body \mathcal{B} .

Thus Eq. (3.6) is replacing Eq. (3.5) and similar replacements take place for other pointwise equalities.

Φ is so chosen that (for all $\phi \in \Phi$) $(\eta\phi)'$ and $\left(\frac{\partial \psi}{\partial q} \phi \right)'$ are $L_2(\Omega)$ functions even if q and η are not differentiable.

A philosophical point should be made whether a microsystem described by the pointwise equations (3.1)–(3.5) does really represent the behavior of the body \mathcal{B} after “patching up” neighbouring small pieces of the body, or should some (and perhaps different) averaging processes be applied to describe the observable behavior of \mathcal{B} .

The arguments in favour of considering only weak solutions of the thermodynamic equations describing the state and the rates thermodynamic processes appear to be irrefutable, unless a complete break is made with tradition, and infinitesimal behaviour is studied using completely rigorous mathematical formulation (obviously in a non-standard version of $\mathcal{R}^3 \times \text{time}$) and then “patched up” in a rigorous manner, stepping up from one galaxy to another in the nonstandard terminology (see [26], Chapter VII).

In the spirit of “weak” interpretation, we shall introduce bilinear products which are analogous with our mechanical example in Sect. 2.

3.1. An example of application

A polymer molecule. An approximate kinetic theory analyses the behaviour of a large molecule by estimating the probability $\tilde{p}(\xi, \eta, \zeta)$ that one end of the molecule may be situated in a neighbourhood of the point (ξ, η, ζ) having the volume dV , in a total volume equal to one, while the other end is fixed. This is accomplished by evoking the random walk formula. Approximate formulas have been obtained in the literature by assuming that the chain consists of rigid links, each link having the same length λ . Introducing the variable $l = n^{\frac{1}{2}}\lambda$, various authors proceed to the limit ($n \rightarrow \infty$, $\lambda \rightarrow 0$, $l = \text{const}$), obtaining the formula

$$p = \tilde{p}/dV = \left(\frac{3}{2l^2\pi} \right)^{3/2} \exp \left\{ - \frac{3r^2}{2l^2} \right\},$$

where $r^2 = \xi^2 + \eta^2 + \zeta^2$ (see for example K. VALANIS [17]).

From the point of view of the internal variable theory, we identify the macroscopic behaviour of the polymer by performing some tests which consist in applying forces to the faces of the test specimen, and recording the response of the test sample.

Since continuum mechanics arguments are used, the validity of the entire argument

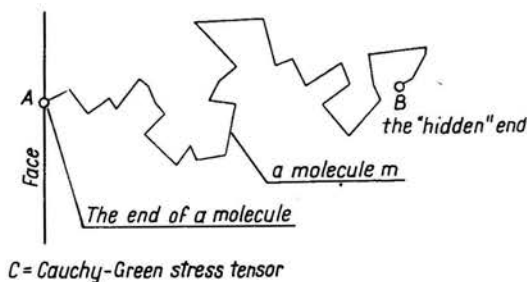


FIG. 3.

must be questioned if the size of the specimen is of the same order of magnitude as the chain element of the molecule.

The point A is the only point along the entire length of the molecule \mathcal{M} at which the stress tensor is observable, whereas the stresses and strains along the length of \mathcal{M} due to the interaction of \mathcal{M} with other molecules must be regarded as internal variables.

Suppose that we denote the displacement along the i -th molecule \mathcal{M}_i to be the internal variable q_i . The forces acting on the molecule \mathcal{M}_i are opposing the motion of the molecule. Hence $g_{ij}\dot{q}_{ij} \leq 0$; (neither i , nor j is summed). The subscript j denotes the j -th coordinate; $j = 1, 2, 3$. Conceptually the situation is similar to the example illustrated in Fig. 1 of Sect. 2.

While the molecule experiences a force field along its entire length, the only observable force is exerted at the point A with the spacial coordinates $\mathbf{x} = \mathbf{x}_0$ situated on the face of the specimen.

A few simplifying assumptions can be made at this point. Let us suppose that the force exerted is purely entropic, and the free energy of the molecule is given by

$$\psi = -k\theta \log p,$$

that is ψ is of the form

$$(3.7) \quad \psi = -3/2 \left\{ k\theta \log \left(\frac{3}{2\pi l^2} \right) \right\} + 3/2 \left\{ k \int_0^l \theta \frac{\|\mathbf{x}_i\|^2}{l^2} ds \right\},$$

where \mathbf{x}_i denotes the position vector along the i -th molecule and k is the Boltzmann constant.

For the sake of simplicity let us consider an isothermal deformation. The force necessary to change the position of the i -th molecule from $\mathbf{x}_i(s)$ to $\mathbf{y}_i(s)$ is given by

$$(3.8) \quad f = 3/2(k\theta/l^2) \int_0^l (\mathbf{x}_i - \mathbf{y}_i)^2 ds.$$

To represent the motion of the system we can introduce a Hilbert space of vectors $\mathbf{u}_{i_1}, \mathbf{u}_{i_2}$, representing different continuous displacements of the i -th molecule. We assign the following weighed L_2 product:

$$\langle \mathbf{u}_1, \mathbf{u}_2 \rangle = \int_0^l (C(s) \mathbf{u}_{1i}(s) \mathbf{u}_{2i}(s)) ds,$$

where $C(s)$ is a positive function. We shall take $C = 3/2(k\pi/l^2) = \text{const}$. We also define

the product $(u_{01} \cdot u_{02})$, where \cdot denotes ordinary multiplication, the numbers u_{01}, u_{02} representing the boundary values of the functions u_1, u_2 on the surface Γ of the specimen. (The subscript i was omitted because of the inconvenience of triple subscripting.) As before the subscripts 1 and 2 denote the first and second mode of displacement, while the subscript i refers to the i -th molecule.

The product (\cdot, \cdot) trivially generates an inner product space H_0 , isomorphic to $R \times R$, representing an ordinary multiplication of the observable displacements on the face Γ of the specimen.

We can now define a product $\{ , \}$ on the inner product space $H_1 \oplus H_0$: $\{u_1, u_2\} = \langle u_1, u_2 \rangle + (u_1, u_2)$. Let $w_i \in H = H_1 \oplus H_2$ represent the displacement of the i -th molecule. The force acting on this molecule is represented by the Fréchet derivative

$$(3.9) \quad f_i(s) = \frac{\partial \Delta \psi}{\partial w_i(s)}.$$

Hence the resistive property of molecular motions is represented by the inequality

$$(3.10) \quad \sum_{i=1}^N \int_0^l \frac{\partial \Delta \psi}{\partial q_i(s)} \cdot \dot{q}(s) ds \leq 0.$$

This result is an analogue of the continuum mechanics equations of the form (1.6).

Adjoining the entropy γ , we can evidently write for the system of N molecules

$$(3.11) \quad \theta \dot{\gamma}_j = - \sum_{j=1}^N \int_0^l \frac{\partial \Delta \psi}{\partial w_j} \dot{w}_j \geq 0,$$

where $w(s) = q(s)$ is the internal variable if $s > 0$, and $w(0) = u_{0j}(x, y)$ is the observable displacement if $s = 0$. Here x, y are restricted to the face of the specimen.

An almost analogous example, which leads to a similar expression, involves a simple quantum mechanical model of the nonlinear field theory, namely the model of a one dimensional elastic chain of atoms subjected to an external field. If time is measured in units of c/ω_1 where ω_1 is the lowest natural frequency, and c is the natural speed of propagation of disturbances (analogous to the speed of sound) then the displacement of the elastic chain in an appropriate limit is described by the linear Klein-Gordon equation

$$(3.12) \quad \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + u = 0,$$

with one end condition: either $\frac{\partial u(0, l)}{\partial x} = 0$, or $u(0, l) = 0$. The other end is free.

Alternatively, the behaviour of this chain is described by the nonlinear equation

$$(3.13) \quad \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + u - |u|^2 \cdot u = 0,$$

with identical end conditions. Equation (3.13) has the following physical interpretation. The displacement u is complex valued. Its real and imaginary parts correspond to displacements in mutually orthogonal directions, the chain being capable not only of transverse vibrations, but also of internal rotations of the molecules. The term $u - |u|^2 \cdot u$ represents

the unobservable interaction due to the elastic bonds between the molecules. At this point most authors make some simplifying assumptions, such as the monochromatic property of the solutions; see for example [29]. In fact the assumption leading to Eq. (3.13) amounts to the specification of the equation of state. The additional monochromatic assumption is equivalent to the uncoupling of the different modes of vibration, so that variables can be separated. A different approach could stipulate that the unobservable dissipative internal rotation of the molecule is represented by an internal variable q , the basic equation of motion assuming the form

$$(3.14) \quad \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + u(1 - |q|^2) = 0, \quad q(0, l) = 0.$$

The complex valued displacements allow us to formulate Eq. (3.13) as a variational equation, corresponding to a stationary behaviour of the functional

$$\|u_x\|^2 - \|u_t\|^2 + \frac{1}{2} \|u\|^2 - 1/4 \|u\|^4,$$

where

$$\|u\| = \langle u, u \rangle_{S, x \in [0, T]}.$$

Introduction of a bilinear product

Let $\{\mathbf{q}_1, \theta_1\}$, $\{\mathbf{q}_2, \theta_2\}$ describe states of a thermodynamic system corresponding to two (possibly different) thermodynamic processes on the time interval (t_0, T) , or (if one specifically recognizes the strain components) $\{\mathbf{q}_1(t), \mathbf{C}_1(t), \theta_1(t)\}$, and $\{\mathbf{q}_2(t), \mathbf{C}_2(t), \theta_2(t)\}$, not identifying them with specific values of q (say at the boundary).

The products defined below are well known in continuum mechanics and appear under names of "mutual compliance". Of course, they are simply "energy products" in the language of mathematical physics. See for example MIKHLIN [10]. The subscript 1 will denote the actual system considered. Subscript 2 denotes "adjoint" system which does not necessarily obey the physical laws of thermodynamics.

We define at time t the product

$$(3.15) \quad \tilde{\psi}_{1,2} = \tilde{\psi}_{1,2}(\mathbf{q}_1, \mathbf{C}_1, \mathbf{q}_2, \mathbf{C}_2) \int_{\mathcal{S}} K(x, \zeta) A_{1,2}(\mathbf{q}_1, \mathbf{C}_1, \mathbf{q}_2, \mathbf{C}_2) dx d\zeta,$$

where $K(x, \zeta)$ is a positive definite symmetric kernel.

$A_{1,2}$ is a symmetric operator

$$(3.16) \quad A_{1,2}(\mathbf{q}_1, \mathbf{C}_1, \mathbf{q}_2, \mathbf{C}_2) = A_{2,1}(\mathbf{q}_2, \mathbf{C}_2, \mathbf{q}_1, \mathbf{C}_1);$$

$\tilde{\psi}_{1,2}$ has the property that

$$(3.17) \quad \tilde{\psi}_{1,1}(\mathbf{q}_1, \mathbf{C}_1, \mathbf{q}_1, \mathbf{C}_1) = \psi(\mathbf{q}_1, \mathbf{C}_1)$$

is the Helmholtz free energy ψ associated with the state $\{\mathbf{q}_1, \mathbf{C}_1\}$.

NOTE 1. θ is regarded here as one of the generalized displacements: \mathbf{q}_{n+1} .

NOTE 2. There is no reason why $K(x, \zeta)$ should not be a history-dependent kernel. For the sake of simplicity in discussing the concepts introduced here, this aspect shall not be stressed.

We also introduce the kinetic energy product

$$(3.18) \quad \tilde{T}_{1,2}(\dot{\mathbf{q}}_1, \dot{\mathbf{C}}_1, \dot{\mathbf{q}}_2, \dot{\mathbf{C}}_2) = \frac{1}{2} \int_{\mathcal{B}} (\varrho(x) \dot{\mathbf{q}}_1 \dot{\mathbf{q}}_2) dx + \frac{1}{2} \int_{\mathcal{B}} \sum_{\alpha\beta\gamma\delta} \gamma^{\alpha\beta\gamma\delta}(x) \dot{C}_{1,\alpha\beta} \dot{C}_{2,\gamma\delta} dx,$$

$\gamma^{\alpha\beta\gamma\delta}$ is a positive definite symmetric matrix. Here we have assumed a single internal variable q , however, the term $1/2 \int_{\mathcal{B}} (\varrho \dot{\mathbf{q}}_1 \dot{\mathbf{q}}_2) dx$ is easily modified otherwise to read

$$(3.19) \quad \frac{1}{2} \int_{\mathcal{B}} \sum_{ij} (\varrho_{ij} \dot{q}_{1i} \dot{q}_{2j}) dx,$$

where ϱ_{ij} is a generalized density matrix. Generally, ϱ_{ij} is a constant diagonal matrix.

The terms (3.18) and (3.19) include θ as one of the internal variables \mathbf{q} . In fact more than one temperature variable could be introduced as the generalized internal variables $\mathbf{q}^t - s$.

We also introduce the product $\tilde{\psi}_{1,2}$ which is defined below.

To identify the form of $\tilde{\psi}_{1,2}$ we introduce a variable S_i , such that $\dot{S}_i = \dot{Q}_i = -\frac{\partial \psi}{\partial q_i}$.

We notice the identifying q_{n+1} with the temperature θ and we have

$$\int^t S_{n+1} dt = -\eta, \quad \text{or} \quad S_{n+1} = -\dot{\eta}.$$

The symmetric product for $n+1$ variable θ is identified as

$$\tilde{\psi}_{1,2(n+1)} = \frac{1}{4} \int_{\mathcal{B}} (S_2 \dot{\theta}_1 + S_1 \dot{\theta}_2) dx$$

(the index $(n+1)$ now being omitted). Hence $\tilde{\psi}_{1,2}$ could be assumed to be of the form

$$(3.20) \quad \tilde{\psi}_{1,2} = \sum_{K=1}^{n+1} (S_{K_2} \dot{q}_{K_1} + S_{K_1} \dot{q}_{K_2}) dx,$$

the subscripts 1, 2 referring to different states.

The total energy is defined as the Hamiltonian $\tilde{H}(t)$ in analogy with classical mechanics.

We define

$$(3.21) \quad \tilde{H}_{1,2}(t) = \tilde{\psi}_{1,2}(t) + \tilde{T}_{1,2}(t)$$

and

$$(3.22) \quad \tilde{\mathcal{L}}_{1,2}(t) = \frac{1}{2} \int_{\mathcal{B}} (\mathbf{p}_1 \dot{\mathbf{q}}_2 + \mathbf{p}_2 \dot{\mathbf{q}}_1) dx + \frac{1}{2} \int_{\mathcal{B}} \Pi_{1,\gamma\delta} C_{2,\gamma\delta} + \Pi_{2,\gamma\delta} C_{1,\gamma\delta} dx - \tilde{H}_{1,2},$$

where p_i, Π_i stands for

$$(3.23) \quad p_i = \frac{\partial \tilde{T}_{1,i}}{\partial \dot{q}_i} = \varrho \dot{q}_i, \quad i = 1, 2,$$

where $q_{n+1} = S_{n+1}$ and

$$(3.24) \quad \Pi_{i\alpha\beta} = \frac{\partial \tilde{T}_{1,i}}{\partial \dot{C}_{i\alpha\beta}} = \sum_{\gamma\delta} \gamma^{\alpha\beta\gamma\delta} C_{i,\gamma\delta}.$$

An internal dissipation function $D(q_1, q_2, \dot{q}_1, \dot{q}_2)$ is now introduced. In the model developed in this paper it is assumed that the dissipation function $D_{1,2}$ due to the internal displacements $\mathbf{q}_1, \mathbf{q}_2$ is of the form

$$(3.25) \quad \tilde{D}_{1,2} = \frac{1}{4} \int_{\mathcal{B}} (\mathbf{q}_1 \mathbf{b} \dot{\mathbf{q}}_2 - \mathbf{q}_2 \mathbf{b} \dot{\mathbf{q}}_1) dx,$$

where $\mathbf{q}_2 = 0$ on $\partial \mathcal{B}$.

Integration by parts yields

$$(3.25') \quad D_{1,2} = \frac{1}{2} \int_{\mathcal{B}} (\mathbf{q}_1 \mathbf{b} \dot{\mathbf{q}}_2) dx.$$

As before it is understood that \mathbf{q}_1 and \mathbf{q}_2 contain more than one component, and the terms on the right hand side of Eqs. (3.25) and (3.25') constitute tensor products.

The Hamiltonian $\tilde{H}_{1,2}$ is defined

$$(3.26) \quad \tilde{H}_{1,2} = \tilde{H}_{1,2} + D_{1,2}$$

and the Lagrangian

$$(3.27) \quad \tilde{\mathcal{L}}_{1,2} = \tilde{\mathcal{L}}_{1,2} - \tilde{D}_{1,2} - \hat{\mathbf{Q}}_1 \dot{\mathbf{q}}_2 - \hat{\mathbf{Q}}_2 \dot{\mathbf{q}}_1,$$

where $\hat{\mathbf{Q}}_1, \hat{\mathbf{Q}}_2$ are internally applied forces.

Let q_j be an internal variable in either state "one" or "two". Then

$$(3.28) \quad \frac{\partial \tilde{\mathcal{L}}_{i,j}}{\partial \mathbf{q}_j} = \frac{\partial \psi}{\partial \mathbf{q}_j} \pm \sum_i \mathbf{b}_{ij} \dot{\mathbf{q}}_i, \quad i, j = 1, 2, \quad i \neq j,$$

where + or - signs apply depending on the state (+ for state "one", - for state "two").

$$\frac{d}{dt} \left(\frac{\partial \tilde{\mathcal{L}}_{ij}}{\partial \dot{\mathbf{q}}_j} \right) = \frac{d}{dt} \left\{ \sum_i \pm \mathbf{b}_{ij} \mathbf{q}_i + \sum_i \varrho_{ij} \dot{\mathbf{q}}_i \right\}, \quad i = 1, 2, \quad i \neq j.$$

Introducing the "vectors" $\mathbf{w}_1, \mathbf{w}_2$,

$$(3.29) \quad \mathbf{w}_i = \{\mathbf{q}_i, \mathbf{C}_i, \theta_i\}$$

and taking a Fréchet derivative of $\mathcal{L}_{1,2}$ with respect to \mathbf{w}_2 or \mathbf{w}_1 , we obtain a system of Euler-Lagrange equations:

$$(3.30) \quad \frac{\partial \tilde{\psi}_{1,2}}{\partial q_2} + \varrho \ddot{\mathbf{q}}_1 + b_{1,2} \dot{\mathbf{q}}_1 = \hat{\mathbf{Q}}_1$$

or more generally a weak form

$$(3.30') \quad \left\langle \phi, \frac{\partial \tilde{\psi}_{1,2}}{\partial \mathbf{q}_{j_2}} + \varrho_{ij} \ddot{\mathbf{q}}_{j_1} + \mathbf{b}_{ji} \dot{\mathbf{q}}_{j_1} \right\rangle - \langle \hat{\mathbf{Q}}_{j_1}, \phi \rangle = 0$$

for all ϕ in a chosen test space \mathcal{D} . $\hat{\mathbf{Q}}_1$ is a generalized force applied directly to some regions in the interior of Ω . $\langle \cdot, \cdot \rangle$ denotes the usual L_2 product in Ω . Similar equations derive for the \mathbf{C}_i -s.

Omitting the subscripts j , we can at this point identify the solutions of the differential equations:

$$(3.31) \quad \frac{\partial \mathcal{L}_{1,2}}{\partial \mathbf{q}_2} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}_{1,2}}{\partial \dot{\mathbf{q}}_2} \right) = \hat{\mathbf{Q}}_1,$$

$$(3.32) \quad \frac{\partial \mathcal{L}_{1,2}}{\partial \mathbf{q}_1} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}_{1,2}}{\partial \dot{\mathbf{q}}_1} \right) = \hat{\mathbf{Q}}_2,$$

as the displacements of the physical system considered, and as the displacements corresponding to an adjoint system, respectively.

Because of the form of the dissipation product $\tilde{D}_{1,2}$, the physical system dissipates energy proportionally to the velocity of the generalized displacements (including temperature!), i.e. we have assumed viscous (or dashpot) type damping.

As is usually the case with non-conservative systems, the adjoint system is marching backward in time, displaying negative dissipation. An interesting observation can be made at this point that $\psi(q)$ can not be an algebraic quadratic form in all variables, contrary to simplistic expectations. If it were so, the following argument could be advanced. Setting $\tilde{\psi}_{1,2} = \int_{\mathcal{A}} (\mathbf{q} \mathbf{K} \mathbf{q}_2) dx$, we would have

$$\frac{\partial \psi_{1,2}}{\partial q_2} = \hat{\mathbf{K}} \mathbf{q}_1,$$

and the internal displacement q_1 obeys a second-order differential equation

$$\langle (\hat{\mathbf{K}} \mathbf{q}_1 + \mathbf{b} \mathbf{q}_1 + \rho \ddot{\mathbf{q}}_1), \phi \rangle - \langle \mathbf{Q}_1, \phi \rangle = 0.$$

If the coefficients $\hat{\mathbf{K}}$, \mathbf{b} , ρ are not functions of time (as would be the case if they were memory dependent), then in the one-dimensional case the classical solution can be easily written down for the case $\hat{Q}_i = 0$, $i = 1, 2$.

Identifying S_{n+1} with $\dot{\eta}$ and using the second law of thermodynamics in the form $\dot{\eta} = -h_{i,i}/\theta$, and ignoring the effects of all other variables on the behavior of the system, we obtain, by differentiating $\psi_{1,2}$ with respect to the second state variable, $\partial \psi_{1,2} / \partial S_2 = \dot{\eta}_1$, Eq. (3.30') in the form

$$(3.10'') \quad -\dot{\eta}_1 + \rho \ddot{\theta}_1 + b \dot{\theta}_1 = 0.$$

Using Fourier's law

$$\begin{aligned} h_i &= -K\theta_{,i}, \\ h_{i,i} &= -\dot{\eta}\theta, \end{aligned}$$

and omitting the subscript "one", Eq. (3.20)₂ becomes

$$-K\theta_{,ii} + b\dot{\theta} + \rho\ddot{\theta} = 0,$$

which is the heat conduction equation with "the wave term". A comment should be made that $\tilde{\psi}_{1,2}$ is not an explicit function of θ . It is a functional and the derivative $\partial \tilde{\psi}_{1,2} / \partial \theta$ has to be regarded as a Fréchet derivative.

NOTE. The functional nature of dependence of the basic energy terms on the generalized forces and displacements is fairly easily justified by considering the Clausius-Duhem ine-

quality. An argument to that effect is offered by C. ERINGEN in [27], (vol. 2), pages 98–99, where he gave an example of constitutive equations of the type

$$\begin{aligned} T(X, t) &= \hat{T}(x, \theta), & \psi(X, t) &= \hat{\psi}(x, \theta), \\ Q(X, t) &= \hat{Q}(x, \theta), & \eta(X, t) &= \hat{\eta}(x, \theta), \\ P(X, t) &= \hat{P}(x, \theta) \end{aligned}$$

and showed that the assumption that the energy terms are functions of the generalized forces and displacements implies isothermal, rigid body behaviour.

3.2. An example

Let us consider a class of perfectly elastic materials obeying the constitutive equations

$$\begin{aligned} T^{KL} &= 2\rho_0 \partial \hat{\psi}(C, \theta) / \partial C_{KL} \quad \text{or} \quad t^{kl} = 2\rho_0 J^{-1} (\partial \psi / \partial C_{KL}) x^k \cdot_{,K} x^l \cdot_{,L}, \\ \eta &= -\partial \hat{\psi}(C, \theta) / \partial \theta, \quad \varepsilon = \hat{\psi} - \theta \partial \hat{\psi} / \partial \theta, \quad Q = 0, \end{aligned}$$

where t^{kl} is the Cauchy stress tensor, T^{KL} is the Piola-Kirchhoff stress (or rather pseudo-stress) tensor, related to t^{kl} by the constitutive relation

$$t^{kl} = 2 \frac{\rho}{\rho_0} \frac{\partial \Sigma}{\partial C_{KL}} x^k \cdot_{,K} x^l \cdot_{,L}.$$

Following some well-known arguments, see for example [28], we can rewrite the constitutive equations in an alternative form:

$$\begin{aligned} T^{KL} &= 2\rho_0 \partial \hat{\varepsilon}(C, \eta) / \partial C_{KL} \quad \text{or} \quad t^{kl} = 2\rho_0 J^{-1} (\partial \hat{\varepsilon} / \partial C_{KL}) x^k \cdot_{,K} x^l \cdot_{,L}, \\ \theta &= \partial \hat{\varepsilon}(C, \eta) / \partial \eta, \quad \psi = \hat{\varepsilon} - \eta \partial \hat{\varepsilon} / \partial \eta. \end{aligned}$$

This system of equations is easily restated in the generalized Hamiltonian form as defined by B. NOBLE [23], and given by Eqs. (4.2)₁ and (4.2)₂ in the next section of this paper, by assuming a simple static form of the Hamiltonian:

$$\tilde{H}_{12} = \frac{1}{2} \{ \langle T_1^{KL}, C_{KL_1} \rangle + \langle \theta_1, \eta_2 \rangle + \langle T_2^{KL}, C_{KL_1} \rangle + \langle \theta_2, \eta_1 \rangle \}.$$

More realistic assumptions would consider some kinetic and dissipation effects.

We can modify the constitutive equations by considering the inertia and dissipation terms derived from the modified Hamiltonian: $H_{12} = \tilde{H}_{12} + T_{12} + D_{12}$, where the kinetic and dissipation functionals are given respectively by

$$\begin{aligned} T_{12} &= \int_{\Omega} (v^{KLMN} \dot{C}_{KL_1} \dot{C}_{KL_2}) dx, \\ D_{12} &= \int_{\Omega} (T_1^{KL} \dot{C}_{KL} + \theta \dot{\eta}) dx. \end{aligned}$$

(We have deliberately omitted the constant term $2\rho_0$, which can be easily absorbed in the definition of the product $\langle \cdot, \cdot \rangle$.) The Hamiltonian H_{12} given above could serve as an illustration for the subsequent discussion offered in Sect. 4 and 5 of this paper.

4. The Hamiltonian formulation and associated variational principles

Formulas (3.12) and (3.13) define the Legendre transformation which introduces the generalized momenta

$$\mathbf{p}_t, \Pi_{t\alpha\beta}$$

and establishes the relation between the Lagrangian and Hamiltonian functionals

$$L_{1,2}(\mathbf{q}_1, \mathbf{q}_2, \mathbf{C}_1, \mathbf{C}_2)_{(B)} = \frac{1}{2} \int_{\mathcal{B}} (\Pi_1 \mathbf{C}_2 + \Pi_2 \mathbf{C}_1) dx - \frac{1}{2} \int_{\mathcal{B}} (\mathbf{p}_1 \mathbf{q}_2 + \mathbf{p}_2 \mathbf{q}_1) dx - H_{1,2},$$

where

$$H_{1,2} = T_{1,2} + \psi_{1,2} + D_{1,2}$$

and where all products $\alpha\beta$ are componentwise sums, i.e.

$$\alpha\beta = \sum_{i=1}^n \alpha_i \beta_i.$$

We obtain directly

$$(4.2) \quad \dot{\mathbf{p}}_1 = \frac{\partial H_{1,2}}{\partial \mathbf{q}_2}, \quad \dot{\Pi}_1 = \frac{\partial H_{1,2}}{\partial \mathbf{C}_2}, \quad \dot{\mathbf{p}}_2 = \frac{\partial H_{1,2}}{\partial \mathbf{q}_1}, \quad \dot{\Pi}_2 = \frac{\partial H_{1,2}}{\partial \mathbf{C}_1};$$

$$(4.3) \quad \dot{\mathbf{q}}_1 = -\frac{\partial H_{1,2}}{\partial \mathbf{p}_2}, \quad \dot{\mathbf{q}}_2 = -\frac{\partial H_{1,2}}{\partial \mathbf{p}_1}, \quad \dot{\mathbf{C}}_1 = -\frac{\partial H_{1,2}}{\partial \Pi_2}, \quad \dot{\mathbf{C}}_2 = -\frac{\partial H_{1,2}}{\partial \Pi_1}.$$

The system (4.2), (4.3) is the complete set of Hamilton's "canonical" equations.

It is equivalent to the vanishing of Fréchet derivatives

$$(4.4)_1 \quad \frac{\partial \mathcal{L}_{1,2}}{\partial \mathbf{q}_2} = \frac{\partial \mathcal{L}_{1,2}}{\partial \mathbf{q}_1} = \frac{\partial \mathcal{L}_{1,2}}{\partial \mathbf{C}_2} = \frac{\partial \mathcal{L}_{1,2}}{\partial \mathbf{C}_1} = 0,$$

$$\frac{\partial \mathcal{L}_{1,2}}{\partial \mathbf{p}_2} = \frac{\partial \mathcal{L}_{1,2}}{\partial \mathbf{p}_1} = \frac{\partial \mathcal{L}_{1,2}}{\partial \Pi_2} = \frac{\partial \mathcal{L}_{1,2}}{\partial \Pi_1} = 0;$$

hence, to the existence of a critical point of the Lagrangian functional $\mathcal{L}_{1,2}$. We summarize Eqs. (4.4)₁ by the variational statement

$$(4.4)_2 \quad \delta \mathcal{L}_{1,2} = 0.$$

In the event when one wishes to obtain the boundary conditions directly from the Lagrangian, one can do so by modifying the Lagrangian. For example, if the boundary conditions are of the form

$$(4.5) \quad \Gamma_1(\mathbf{q}_t, \mathbf{C}_t) = 0 \quad \text{on} \quad \partial\Omega \quad \text{at} \quad t = 0,$$

then, one can introduce an additional term

$$H_{1(\partial\Omega \times 0)} = p_2 \Gamma_1(\mathbf{q}, \mathbf{C})_{(\partial\Omega \times 0)}$$

into the Hamiltonian, and a corresponding term $p_q \dot{\mathbf{q}}_{1(\partial\Omega \times 0)} - H_{1(\partial\Omega \times 0)}$ into the Lagrangian. Suppose this modified Lagrangian assumes a stationary value. Extending the Fréchet differentiation to functions defined on Ω and continuously extended to $(\partial\Omega \times 0)$ completes

this development, whereby a critical point of the modified Lagrangian $\mathcal{L}_{1,2}$ yields simultaneously the set of equations (4.2)–(4.3) and the boundary condition (4.5). It is easily seen that other initial boundary conditions could be handled by a similar set of tricks. See original ideas presented in [7] or a more recent development in [2].

The condition that $\mathcal{L}_{1,2}$ attains a maximum or a minimum (or neither) is completely determined by the nature of the operators defined as the second Fréchet derivatives of the Hamiltonian $H_{1,2}$.

For example we can check the behaviour of

$$\frac{\partial^2 H_{1,2}}{\partial q_{n+1}^2} = \frac{\partial^2 H_{1,2}}{\partial \theta^2} = \frac{\partial \eta_2}{\partial \theta_2} + \frac{\partial \eta_1}{\partial \theta_1}.$$

If we hypothesise that $\eta(\theta)|_{\mathbf{q}, \mathbf{C}=\text{const}}$ is a monotone function, then the existence of a support hyperplane follows, and keeping \mathbf{C} , \mathbf{q} constant $\mathcal{L}_{1,2}$ attains an extreme value at the point in Hilbert space if and only if Eqs. (4.2) and (4.3) are satisfied.

The dual variational principles associated with Hamiltonian systems of the type (4.2), (4.3) are well known. However, in general, the dissipation terms will cause problems concerning the sign of the second Fréchet derivatives, and only a set of necessary conditions for the existence of a maximum or a minimum can be formulated in the general case for the Lagrangian $\mathcal{L}_{1,2}$, unless additional information is given concerning relations between the variables q, \dot{q}, C, \dot{C} , etc. In fact to determine the extremal behaviour of the Lagrangian, we need in addition to Eqs. (4.2) and (4.3) a set of constitutive equations.

If we assume that the Hamiltonian system (4.2), (4.3) is deterministic, then, given a sufficient number of initial conditions, the system (4.2), (4.3) can be solved, provided the function $H_{1,2}$ is known. Of course, the problem arising in material science is the inverse problem. $H_{1,2}$ is not supplied in advance. Instead, due to some experimentation and/or guesswork some relations are given between the variables $\mathbf{q}, \mathbf{C}, \dot{\mathbf{q}}, \dot{\mathbf{C}}$, and $H_{1,2}$, $\mathcal{L}_{1,2}$ are derived or guessed by us, so that the system (4.2) agrees with the experimental findings. This is sometimes difficult to achieve. As an example consider the simplest form of Hooke's law

$$\frac{\partial H_{1,2}}{\partial \mathbf{C}_1} = \mathbf{K} \cdot \mathbf{C}_2 \quad (\mathbf{K} \cdot \mathbf{C}_2 \text{ stands for } K_{ijkl} C_{2kl}).$$

This agrees with Eq. (4.2)₄ only if we postulate Newton's second law

$$\rho \cdot \dot{\mathbf{\Pi}} = \mathbf{K} \cdot \mathbf{C}, \quad \text{i.e.,} \quad \rho \dot{I}_2 = \mathbf{K} \cdot \mathbf{C}_2.$$

This introduction of Newton's law is not really objectionable, but it must be regarded with suspicion by anybody trained in the classical theory of elasticity. In fact, it appears that the system (4.2) does not provide sufficient flexibility to encompass most classical theories.

However, generalization of Eq. (4.2) exists and we could adapt a scheme originally proposed by B. NOBLE (see [23], RALL, [13], KOMKOV [6], [7]), and suggest the following representation which is best explained in a Hilbert space setting.

Let T be an operator mapping a Hilbert space of functions H_1 into a Hilbert space H_2 . The domain of T is dense in H_1 , and consequently the operator $T^*: H_2 \rightarrow H_1$ is de-

fined. T^* will be only a formal adjoint of T in this discussion. Suppose a Hamiltonian functional \hat{H} can be found $\hat{H}(H_1, H_2)$ such that for the suitable functions $\phi \in H_1, p \in H_2$,

$$\frac{\partial \hat{H}}{\partial \phi} = T^*p \quad (\text{in } \Omega),$$

$$\frac{\partial \hat{H}}{\partial p} = T\phi \quad (\text{in } \Omega)$$

domain of

$$\phi = \Omega \subseteq R^n;$$

domain of

$$p = \Omega \subseteq R^n,$$

$$\sigma_\beta(\phi) = \phi_\beta \quad \text{on} \quad \partial\Omega,$$

are satisfied.

Then $\{\phi, p\}$ is the critical pair of $\hat{\mathcal{L}}$ where

$$\mathcal{L} = \langle \phi, T^*p \rangle_\Omega - \mathcal{H}(\phi, p) + (p, \sigma_\beta(\phi))_{\partial\Omega}$$

while \langle, \rangle denotes the inner product in H_1 ; $(,)_{\partial\Omega}$ is the boundary bilinear form.

It turns out that the Hilbert space setting is unnecessary, and no change in this theory is required if other bilinear forms are substituted, such as convolution products. (See GURTIN's article [11], or [12]).

5. A more general variational formulation

Following the ideas of [23, 6, 13], we could consider more general forms of the Lagrangian $\mathcal{L}_{1,2}$ and the Hamiltonian $H_{1,2}$.

Suppose that the internal variables \mathbf{q}_i and the components of the strain tensor $\mathbf{C}_{\alpha\beta}$ are elements of a Hilbert space H of functions whose domain is \mathcal{B} . A, B, δ and η are linear operators mapping H into H ; the domains of A, B, δ, η are dense in H . A and B are normal operators. Define

$$T_{1,2}(A\mathbf{q}_1, BC_1, A\mathbf{q}_2, BC_2),$$

$$D_{1,2}(A\mathbf{q}_1, \mathbf{q}_2, BC_1, C_2)$$

to be

$$T_{1,2} = \frac{1}{2}[\langle A\mathbf{q}_1, A\mathbf{q}_2 \rangle + \langle BC_1, BC_2 \rangle],$$

$$D_{1,2} = \frac{1}{4}[\langle \delta\mathbf{q}_1, \mathbf{q}_2 \rangle + \langle \eta C_1, C_2 \rangle] + \frac{1}{4}[\langle \mathbf{q}_1, \delta^*\mathbf{q}_2 \rangle + \langle C_1, \eta^*C_2 \rangle].$$

As before $\psi_{1,2}$ depends on the variables $\mathbf{q}_1, \mathbf{q}_2, C_1, C_2$.

We define again the total energy to be

$$H_{1,2} = \psi_{1,2}(t) + T_{1,2}(t).$$

The momenta are defined as before

$$(5.1) \quad p_i = \frac{\partial T_{i,t}}{\partial(Aq_i)},$$

$$\Pi_{i\alpha\beta} = \frac{\partial T_{i,t}}{\partial(BC_{i\alpha\beta})}$$

and the Lagrangian

$$\mathcal{L}_{1,2} = \langle \mathbf{p}_1, Aq_2 \rangle + \langle \mathbf{\Pi}_1, BC_2 \rangle - (H_{1,2} + D_{1,2}).$$

Then the vanishing of the Fréchet derivatives given by Eqs. (4.4)₁ and (4.4)₂ is equivalent to the generalized Hamiltonian system. Denoting by $\tilde{H}_{1,2} = H_{1,2} + D_{1,2}$ we obtain

$$(5.2) \quad A^*p_i = \frac{\partial \tilde{H}_{1,2}}{\partial q_2}, \quad B^*\Pi_i = \frac{\partial \tilde{H}_{1,2}}{\partial C_2}, \quad A^*p_2 = \frac{\partial \tilde{H}_{1,2}}{\partial q_1}, \quad B^*\Pi_2 = \frac{\partial \tilde{H}_{1,2}}{\partial C_1};$$

$$(5.3) \quad Aq_1 = \frac{\partial \tilde{H}_{1,2}}{\partial p_2}, \quad Aq_2 = \frac{\partial \tilde{H}_{1,2}}{\partial p_1}, \quad BC_1 = \frac{\partial \tilde{H}_{1,2}}{\partial \Pi_2}, \quad BC_2 = \frac{\partial \tilde{H}_{1,2}}{\partial \Pi_1}.$$

This is a complete system of generalized equations of Hamilton describing the behaviour of the physical system, and of the adjoint system.

This reduces to the equations of motion of the form (3.20) and to the adjoint equations if $A = B = \delta = \eta = \frac{d}{dt}$.

5.1. An example: The Onsager-Machlup theory

Following the basic papers of L. ONSAGER and S. MACHLUP [30, 31] one could form an analogy between irreversible thermodynamic phenomena and quantum mechanical behaviour of particles in a Coulomb gauge. The macroscopic variables follow the Onsager paths corresponding to a minimum value of a functional related to the entropy production of the system. The part played by \hbar in quantum mechanics is assumed in this theory by the Boltzmann constant k . If one assumes that the evolution equation for the macroscopic processes is of the form

$$\dot{\alpha}_i = G_i(\alpha_i) + F_i(t),$$

where α_i are the macroscopic variables, G_i are functions of α_i which are assumed linear in the Onsager-Machlup theory, and F_i are random fluctuations with a zero mean value. According to Onsager and Machlup, $\alpha(t)$ follows a path which minimizes a functional of α and $\dot{\alpha}$ in a manner analogous to the minimization of the action integral in classical quantum mechanics. By assuming the random fluctuations to be Gaussian, the Onsager-Machlup theory leads to the Fokker-Planck equation for conditional probability

$$P(\alpha, \alpha_0, t-t_0) = \exp(-S/k), \quad S = S(\alpha, t),$$

where S is the solution of a corresponding Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \sum_i G_i \frac{\partial S}{\partial \alpha_i} + \frac{1}{2} \sum_{i,j} R_{ij} \frac{\partial S}{\partial \alpha_i} \frac{\partial S}{\partial \alpha_j} = k \left[\frac{1}{2} \sum_{i,j} \frac{\partial^2 S}{\partial \alpha_i \partial \alpha_j} R_{ij} + \sum_i \frac{\partial G_i}{\partial \alpha_i} \right],$$

which in the first order of approximation becomes

$$\frac{1}{2} \sum_{i,j} R_{ij} \frac{\partial S^0}{\partial \alpha_i} \frac{\partial S^0}{\partial \alpha_j} + \sum G_i \frac{\partial S^0}{\partial \alpha_i} + \frac{\partial S^0}{\partial t} = 0.$$

(See BYUNG CHANG EU [32] with credit given to N. HASHITSUME [33] for the derivation of these equations) where R_{ij} are the coefficients related to the diffusion coefficients α_{ij} by the simple relation

$$R_{ij} = \frac{l}{k} \sigma_{ij},$$

$$\sigma_{ij} \delta(t-\tau) = \langle F_i(t), F_j(\tau) \rangle.$$

Following [32] we could define

$$A_i = \sum_j (\mathcal{R}^{-1})_{ij} G_j,$$

$$\psi = \sum_{i,j} (\mathcal{R}^{-1})_{ij} G_i G_j.$$

We introduce simultaneously with the physical variables α_i the adjoint (unphysical) variables β_i , and formulate the dual Hamiltonina $\kappa_{1,2}$ as follows.

We define the momenta

$$\Pi_{\beta_i} = \frac{\partial S^0}{\partial \alpha_i}, \quad \Pi_{\alpha_i} = \frac{\partial S^0}{\partial \beta_i}.$$

We can copy the Onsager-Hashitsume derivation of a Hamiltonian by offering

$$\kappa_{1,2}(\alpha, \beta, \Pi_\alpha, \Pi_\beta) = \frac{1}{4} \left\{ \sum_{i,j} [R_{ij}(\Pi_{\alpha_i} + A_i)(\Pi_{\beta_j} + B_j) + R_{ij}(\Pi_{\beta_i} + B_i) \right. \\ \left. \times (\Pi_{\alpha_j} - A_j)] - \Psi(\alpha, \beta) \right\},$$

where

$$\Psi(\alpha, \beta) = \sum_{i,j} (R^{-1})_{ij} [G_i H_j + G_j H_i],$$

$\kappa_{1,2}$ satisfies the canonical equations

$$\frac{d\Pi_{\alpha_i}}{dt} = -\frac{\partial \kappa_{1,2}}{\partial \beta_i}, \quad \frac{\partial \Pi_{\beta_i}}{dt} = -\frac{\partial \kappa_{1,2}}{\partial \alpha_i}, \quad \frac{d\alpha_i}{dt} = \frac{\partial \kappa_{1,2}}{\partial \Pi_{\beta_i}}, \quad \frac{d\beta_i}{dt} = \frac{\partial \kappa_{1,2}}{\partial \Pi_{\alpha_i}}.$$

If the quantities α, β are regarded as elements of a suitable Hilbert space, then the quantities H_i, B_i are defined by the equalities

$$-\left\langle \frac{d\alpha_i}{dt}, \beta \right\rangle = \langle \alpha, H(\beta) \rangle,$$

$$B_i = (R^{-1})_{ij} H_j.$$

The Lagrangian generalizing the Onsager function is given by

$$\mathcal{L}_{12} = \sum_i (\Pi_{\alpha_i} \dot{\beta}_i + \Pi_{\beta_i} \dot{\alpha}_i) - \kappa_{1,2}.$$

Appendix. 1. Infinitesimal calculus in Hilbert spaces

1.1. Parametrized curves and integration

H will denote a Hilbert space which shall be identified as a space of functions with an inner product $\langle \cdot, \cdot \rangle$. By a parameterized curve (curve segment) Γ we mean a continuous map $f: I \rightarrow H$, where I is the unit interval $(0, 1)$. The curve Γ is said to have end points $h_0, h_1 \in H$ if $f(0) = h_0, f(1) = h_1$. It is called simple if for any $\alpha \in (0, 1)$ $f(\alpha)$ is single valued, i.e. $\alpha, \beta \in (0, 1)$ and $\alpha \neq \beta \rightarrow f(\alpha) \neq f(\beta)$. A parametrized curve $\Gamma(\lambda)$ is closed if $f(0) = f(1)$. It is differentiable if for sufficiently small values of $\Delta\lambda = \lambda_1 - \lambda_2$, we have $f(\lambda_1) - f(\lambda_2) = h_1 - h_2 = f'(\lambda)\Delta\lambda + \zeta$ where $f'(\lambda)$ is a (parameterized) vector in H , λ is any value of λ in (λ_1, λ_2) and (the remainder) vector ζ has the property

$$\lim_{|\Delta\lambda| \rightarrow 0} \frac{\|\zeta\|}{|\Delta\lambda|} = 0, \quad \text{i.e.,} \quad \|\zeta\| = o(\Delta\lambda).$$

A straight line segment containing end points h_0, h_1 is a parameterized curve of the form $f(\lambda) = \lambda h_1 + (1 - \lambda)h_0$. Clearly $f'(\lambda)$ is the constant vector $h_1 - h_0$, the remainder term being identically equal to the zero vector. Usually the domain of the functions in H is some subset Ω of \mathcal{R}^r . Ω is regarded as fixed in the discussion of derivatives or integrals of the elements (i.e. functions of H). Suppose that the product $\langle f, g \rangle, f \in H, g \in H$ is defined as the integral

$$\int_{\Omega} W(\mathbf{x})f(\mathbf{x})g(\mathbf{x})d\mathbf{x},$$

where $W(\mathbf{x}) > 0$ in Ω is a weight function. Then the following statement which we label Lemma 1 is easily proved. (Simply apply the Cauchy-Schwartz inequality!)

LEMMA 1. Let $\Gamma(\lambda)$ be a parametrized differentiable curve in H . $\Gamma(\lambda) = f(0, 1)$. Then $f'(\lambda) \in H$ for all $\lambda \in (0, 1)$.

We define the Riemann integral along the parameterized curve $\Gamma(\lambda) \in H$ to be the limit of the Darboux sum

$$\lim_{\Delta\lambda_i \rightarrow 0} \sum_{i=1}^n f(\lambda_i)\Delta\lambda_i = \int_{\Gamma} f(\lambda)d\lambda, \\ (\Delta\lambda_i = \lambda_{i+1} - \lambda_i > 0).$$

LEMMA 2. For any parameterized curve $\Gamma(\lambda)$ the integral $\int_{\Gamma} f(\lambda)d\lambda$ exists.

Outline of proof. This is a direct consequence of the continuity of $f(\lambda)$. Observe $\|\sum f(\lambda_i)\Delta\lambda_i\| < \Sigma \|f(\lambda_i)\|\Delta\lambda_i < \infty$. Now use continuity of f to show that it is impossible to have more than one limit point for the Darboux sum. To show that at least one limit point exists, assume the contrary, and obtain a contradiction to $\Sigma \|f(\lambda_i)\|\Delta\lambda_i < \infty$.

LEMMA 3. Let $f(\lambda), g(\lambda)$ be two parameterized curves Γ_1, Γ_2 in H .

If

$$(A.1.1) \quad F(\lambda) = \langle f(\lambda), g(\lambda) \rangle_{f, g}$$

is defined for each value of λ , then

$$(A.1.2) \quad \int_0^1 F(\lambda) d\lambda = \lim_{\Delta\lambda_i \rightarrow 0} \sum_i F(\lambda_i) \Delta\lambda_i = \lim_{\Delta\lambda_i \rightarrow 0} \sum_i \langle f(\lambda_i), g(\lambda_i) \rangle \Delta\lambda_i.$$

PROOF. Trivial — (Observe that $F_{1,2}$ is a real valued continuous function, the real variable λ). There is no reason why in general the equality

$$(A.1.3) \quad \int_1^0 F(\lambda) d\lambda = \left\langle \int_1^0 f(\lambda) d\lambda, \int_0^1 g(\lambda) d\lambda \right\rangle$$

should be true for arbitrary functions $f(\lambda), g(\lambda)$.

If

$$(A.1.4) \quad f(\bar{x}+th) - f(\bar{x}) = tf'_{\bar{x}}(h) + \zeta(\bar{x}, h), \quad \zeta = o(h),$$

where $f'_{\bar{x}}$ is continuous (in h), then $f'_{\bar{x}}$ is called the Fréchet derivative. (This is not a uniformly accepted definition.) In a Hilbert space the Riesz representation theorem is applicable and $f'_{\bar{x}}(h)$ can be written (for a fixed h) as a product $f'_{\bar{x}}(h) = \langle Df_{\bar{x}}, h \rangle$.

Then $Df_{\bar{x}} \in H$ is frequently referred to as the Fréchet derivative of f at the point \bar{x} .

However, the concept of differentiation given by formula (A.1.4) has been introduced in arbitrary normed spaces E, F and does not require Hilbert space structure. What we require is the existence of a bilinear representation for $f'_{\bar{x}}(h)$. (See [11]). $f'(h) = \langle h, z \rangle$, where z is unique and independent of h . In many works z is defined as the Fréchet derivative of f with respect to x at the point $x = \bar{x}$. This can be generalized to arbitrary bilinear forms, or to arbitrary normed spaces. Let β denote a linear normed space, and β^* its topological dual. Let $x \in \beta, f \in \beta^*$, i.e. $f: \beta \rightarrow \mathcal{R}$ (linearly and continuously).

If $f(\bar{x}+th) - f(\bar{x})$ can be written as

$$f(\bar{x}+th) - f(\bar{x}) = t\phi(h) + \zeta(\bar{x}, th)$$

where $\phi \in \beta^*$ and

$$\lim_{t \rightarrow 0} \frac{\|\zeta\|}{\|th\|} = 0$$

for every h , then ϕ can be denoted as $f'_{\bar{x}}$ and can be designated as the derivative of f at \bar{x} . The Fréchet derivative of a bilinear product $\{u, v\}$, if u, v are regarded as independent, is easily computed since

$$\{u+th, v\} - \{u, v\} = \{th, v\} = t\{h, v\}.$$

However, if the parameterized path $\Gamma(\lambda)$ is restricted to a finite dimensional subspace of H , then Fubini's theorem can be applied directly and the equality (A.1.3) is valid.

We define the line integral $F_{f,f'}$ of the bilinear product $\langle f(\lambda), f'(\lambda) \rangle$ to be the circulation of $f(\lambda)$ along Γ .

Let N be an operator whose domain is H . Following TONTI [25] we define the circulation of $N(f(\lambda))$ along Γ to be

$$\int_{\Gamma} \langle N(f(\eta)), f'(\lambda) \rangle d\lambda.$$

The problem arises whether an equation $Au = f$ in a Hilbert space H can be derived by Fréchet differentiation of a potential functional $F(u)$. The partial answer can be found in [20] and also in [7, 13]. The expected answer is the independence of path Γ of circulation along Γ of $(Au - f)$. This is hinted in the notes [22] and in a very formal fashion obtained in [25].

This theory breaks down non-self adjoint operators, and a flat statement is made in [25] that no potential exists, for example, for the equations $N(u) = f(u, u')$.

On the other hand, there exist known variational principles for such equations. The insistence on Hilbert space setting was questioned by HERRERA and BIELAK [12] who pointed out that the Fréchet differentiation yields identical formulation for arbitrary bilinear products, and the insistence on the inner product space structure only hinders a consistent development of the theory.

1.2. The Fréchet and Gateaux differentiation

Let E, F be any normed (Banach) spaces. Then a map $f: E \rightarrow F$ is called Gateaux differentiable at \bar{x} if for any $h \in E$, and $\bar{x} \in E$, such that for all constants t the vector $x + th \in D(f)$ (the domain of f).

For sufficiently small values of $t \in \mathcal{R}$ we have by bilinearity of the Gateaux derivative $\{, \}$. Hence, using our previous definition $\{u, v\}_u = v$. Using similar arguments, one obtains for a linear map $A: \{Au, v\}_u = A^*v$ provided A^* is defined. For an arbitrary function

$$f \in C^1(V) \quad (u \in V) \quad \{f(u), v\}_u = f'(u) \cdot v,$$

if $\frac{\partial f(u)}{\partial u}$ is defined.

Generally if \mathbf{f}, \mathbf{u} are vectors in a Hilbert or Banach space, $\partial \mathbf{f} / \partial \mathbf{u}$ is a tensor product. If \mathbf{f}, \mathbf{u} are n -dimensional vectors, $\partial \mathbf{f} / \partial \mathbf{u}$ is the Jacobian matrix.

Appendix 2

Some concepts from functional analysis.

The Schwartz space $\mathcal{D}(\Omega)$ is the same as $C_0^\infty(\Omega)$. Here $C_0^\infty(\Omega)$ denotes functions whose support Ω is compact and each function $f \in C_0^\infty$ has derivatives of any (arbitrary) order in Ω . u has derivatives of order α in the weak sense if

$$(A.2.1) \quad \int_{\Omega} u D^\alpha \phi dx = (-1)^{|\alpha|} \int_{\Omega} v \phi dx$$

for some locally integrable function $v \in \Omega$, D^α is the usual multi-index notation

$$A_\alpha \cdot D^\alpha = \sum_{\alpha_1 + \alpha_2 + \dots + \alpha_n = |\alpha|} A_{\alpha_1 \alpha_2 \dots \alpha_n} D^{\alpha_1} D^{\alpha_2} \dots D^{\alpha_n},$$

where $D^j = \frac{\partial^j}{\partial x_j}$. The locally integrable function v in (A.2.1) is called the weak derivative of u , (i.e. $D^\alpha u = v$) if for any $x \in \Omega$ there exists a neighbourhood N_x of such that (A.2.1) holds and $\int_{N_x} v^p dx$ exists. Let $C_p^j(\Omega)$ denote the set of functions such that $u \in C_p^j$ if $\sum_{|\alpha| \leq j} \int_{\Omega} |D^\alpha u|^p dx$ exists.

$$(A.2.2) \quad \|u\|_{j,p} = \left\{ \sum_{|\alpha| \leq j} \int_{\Omega} |D^\alpha u|^p dx \right\}^{1/p}$$

is a norm if $f \leq p < \infty$, and Ω is a bounded domain in R^n . The space $H^{j,p}(\Omega)$ is the Banach space obtained from the closure of C_p^j with respect to the $\|\cdot\|_{j,p}$ norm. The Sobolev space $W_p^j(\Omega)$ is a space of all functions having all weak derivatives up to order j in Ω , where all such derivatives belong to $L^p(\Omega)$. A norm in W_p^j is defined by the formula (A.2.2).

THEOREM

$$W_p^j(\Omega) = H^{j,p}(\Omega).$$

NOTE. If $p = 2$, the index 2 is omitted in this notation. Hence $W_2^j = W^j = H^j$. W_p^j are called the Sobolev spaces. If different orders of weak differentiability are required (if, for example, $u(x, y)$ needs to be twice (weakly) differentiable with respect to x but only once with respect to y), an appropriate Sobolev space can be introduced: $W_p^{2,1}$ the space of functions $u \in W^{2,1}$ whose weak derivatives $\frac{\partial u}{\partial x}$, $\frac{\partial u}{\partial y}$, $\frac{\partial^2 u}{\partial x^2}$ are elements of $L^p(\Omega)$.

The uses of Sobolev spaces in problems of mathematical physics are outlined in MIKHLIN's monograph [10]. For an extensive study of their properties a number of excellent monographs are available, for example A. FRIEDMAN [*Partial differential equations*, R. E. Krieger Publ. Co., Huntington, New York 1976].

Conclusions

This paper accomplishes a twofold purpose. First, the internal variable description of thermodynamic processes of continuum mechanics is generalized from a discrete to the continuous case. The internal variables are pointwise defined continuous functions. Appropriate definitions of Fréchet derivatives generalize the Euler-Lagrange equations. Some simple examples are offered to illustrate the physical interpretation of these concepts. Secondly, a novel formulation is given of Hamilton's canonical equations for irreversible processes, based on a physical-unphysical duality, the physical process, and its unphysical dual corresponding to a stationary behavior of a joint Lagrangian.

"The missing link" between the classical mechanics and the irreversible thermodynamics of continua is provided by the introduction of a kinetic energy and a dissipation term into the free energy of the system.

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