

Variational theory for thermodynamics of thermal waves

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(Received 1 August 2001; revised manuscript received 27 December 2001; published 8 April 2002)

We discuss description of macroscopic representations of thermal fields with finite signal speed by composite variational principles involving suitably constructed potentials along with original physical variables. A variational formulation for a given vector field treats all field equations as constraints that are linked by Lagrange multipliers to the given kinetic potential. We focus on the example of simple hyperbolic heat transfer, but also stress that the approach can be easily extended to the coupled transfer of heat, mass, and electric charge. With our approach, various representations may be obtained for physical fields in terms of potentials (gradient or nongradient representations). Corresponding Lagrangian and Hamiltonian formalism can be developed. Symmetry principles yield components of the energy-momentum tensor for the given kinetic potential. The limiting reversible case appears as a special yet suitable reference frame to describe irreversible phenomena. With the conservation laws resulting from the least action principle and the Gibbs equation, the variational scheme of nonequilibrium thermodynamics follows. Its main property is abandoning the assumption of local thermal equilibrium.

DOI: 10.1103/PhysRevE.65.046132

PACS number(s): 05.70.Ln, 44.10.+i, 47.27.Qb

I. INTRODUCTION

This paper deals with thermal processes described as fields; it is motivated by the fact that the construction of variational principles for irreversible fields still seems to have large difficulties. The most severe difficulty arises from unknown kinetic potentials, which are integrands of functionals that should be extremized, as there are hardly any systematic rules to obtain suitable functions of this sort. Equations of dissipative fluid mechanics and irreversible thermodynamics provide a frequently used Eulerian or field representation of the process. At best, only some truncated forms of these equations were shown to possess the well-known structure of the Euler-Lagrange equations of the classical variational problem [1,2].

When investigating thermal fields two general frameworks may be applied. The first deals directly with differential equations describing the process, whereas the second uses the corresponding action integrals. By extremizing these integrals, solutions of the differential equations in question can be found by the so-called direct variational methods [1]. The important physical ingredient comes with conservation laws obtained from the Hamiltonian actions and symmetry principles [2]. However, for irreversible processes, there are serious impediments to find a general variational formulation. These are attributed to the presence of non-self-adjoint operators [3]. The non-self-adjoint operators cause nonsymmetric Frechet derivatives in the original state space so that according the Vainberg's theorem, an exact variational formulation cannot be found in this space [4,5].

Among the recent results found in the first framework

(differential equations) we stress those obtained during 1985–1997 by Grmela and co-workers. They worked out the so-called bracket formalisms (Grmela [6]; Grmela and Ottinger [7]), the main features of which were exposed in a recent book by Beris and Edwards [8]. The single-bracket and two-bracket descriptions are usually distinguished. These formalisms produce evolution equations via Poissonian and dissipative brackets, the latter being the functional extension of the Rayleigh dissipation function. Yet these bracket approaches are usually not associated with an extremum of a definite quantity. For this purpose a single Poissonian bracket and a Hamiltonian system are both necessary and sufficient.

Working within the variational framework, we focus here on the so-called exact variational formulations, i.e., those that do not involve any subjectively chosen “frozen” variables. These formulations have many well-established virtues. First, physical insight is gained when a single scalar quantity is found that generates the whole vector field represented by many equations of motion. Second, unification of diverse processes is often possible, for example, mechanical, electrical, and even chemical processes. Third, with the so-called direct variational methods that use trial functions, approximate solutions can be obtained. They are usually of good accuracy [1], and they may be the only usable solutions when the analytical solution of the differential equations of interest cannot be found. Fourth, integrals of motion and conservation laws can be obtained from the symmetry principles [2].

In our approach, the process is transferred to a different, suitable space, and a variational formulation is found in that space. This is made by means of certain potentials, similar to those known for electromagnetic field. The origin and properties of these potentials are not explained sufficiently well to date. Our purpose is to contribute to improved understanding of this issue. We exploit some observations done in earlier works on thermal fields [9–11]. We also refer to results obtained for reversible systems, in particular those of Herivel

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[12], Stephens [13], Seliger and Whitham [14], Atherton and Homsy [15], Caviglia [16], and Sieniutycz and Berry [17]. These latter papers proved the crucial role of the Lagrange multipliers in constructing potential representations of physical fields for the purpose of variational principles (see also, Refs. [18,19]).

II. LAGRANGE MULTIPLIERS AS ADJOINTS AND EXTRA VARIABLES IN IRREVERSIBLE PHENOMENA

For nonconservative and other irreversible phenomena, the difficulties in finding variational formulations are attributed to the presence of the so-called non-self-adjoint operators. They introduce asymmetries in the related equations, whence, according to Vainberg's theorem, a suitable functional cannot be found in the space of original variables. We show that these difficulties do not appear when the process space is enlarged by addition of suitable new variables, often called "the potentials," which are, in fact, the Lagrange multipliers for the given constraints. In brief, our method transfers the problem to the space composed of original variables and potentials. In fact, the method assures a spontaneous transfer to the most proper space. The method is easy to apply because the equations for which a variational principle is sought are simply adjoined by Lagrange multipliers (vector λ) to the accepted kinetic potential L .

Yet, to date, the origins and key aspects of approaches of this sort were not enunciated clearly in the literature. Their essence is that the kinetic potential L can be arbitrary, or correct formulations can be found for an infinite number of various L . Until now, this was not stated sufficiently clearly in the literature, perhaps due to the apparent puzzle of a nonunique L . However, a change in the kinetic potential L leaves the original equations unchanged. While this is as it should be, extremum conditions of the action with respect to the original variables do change with changes in L . Whenever the original variables are expressible in terms of the Lagrange multipliers λ , explicit "representations" of the original fields in terms of λ and its derivatives are obtained. They depend on the accepted kinetic potential L , although similar representations could be found for a different L . The new fields λ are adjoint variables for the problem; they "represent" the original variables in the way depending on properties of the original equations and the accepted L . In fact, one can produce an infinite number of different, still correct, representations of the process in the space of the original coordinates and Lagrange multipliers.

In different branches of science, the latter are called by various names. The names adjoint variables or simply adjoints appear as a rule in various problems of optimal control in which the adjoints are companions of original coordinates of state, for any chosen objective function. In some cases the whole variational description can be accomplished only in the space of adjoints; in others, only in the space of original variables. Yet, in the general case, the variational description can be set only in the general composite space of physical variables and their adjoints. In the optimization theory, and in particular in Pontryagin's principle, the role of adjoints is well known. The case of adjoints may also be referred to

variational principles of classical (nonfrictional) mechanics with space coordinates as original variables and momenta as adjoints. It is also worth stressing that the potentials (multipliers, adjoints, momentum-type coordinates, etc., whatever we call them) are quantities of the same sort as those used by Clebsch in his representations of hydrodynamic velocity. Clearly, the phase space, which is well known in the statistical mechanics, is the space composed of the space coordinates and their adjoints.

With all these examples, it should not be surprising that general variational formulations should be sought in extended spaces (with adjoints) rather than in original spaces of physical formulations. The apparent, formal peculiarity of irreversible processes could be accepted in this context only in the way that they require the whole composite space for their variational formulation, meaning that the reduction of coordinates is impossible. From a physical perspective, "irreversibility" can be interpreted to mean that there are some degrees of freedom into which otherwise-conserved quantities such as energy may flow but from which no return can be observed, at least under the conditions of the description or observation. One way to do this is to treat some degree of freedom as implicit rather than explicit. Still, the impossibility of reducing the space seems to be an essential consequence stemming from the presence of both even and odd time derivatives in equations describing the irreversible phenomena.

In the (enlarged) space with Lagrange multipliers or process adjoints as extra coordinates, the difficulties related to asymmetries do not appear. In the realm of the enlarged space, irreversibility properties do little to hamper a variational formulation; they only cause a more complex representation of physical fields for the same L . The dimension of the enlarged space is $2n$, where n is the number of both the original physical variables and the original equations written in the form of first-order (partial or ordinary) vanishing constraints, $C=0$. This is the dimension of what we call here "the proper enlarged space" as the space that is capable of accommodating a variational formulation for every set of first-order differential equations. Spaces of lower dimensions are in general too restricted for that purpose, spaces of larger dimensions are unnecessary. In fact, the proper enlarged space is the space of minimal dimensionality in which a variational formulation still exists for nontruncated equations. In the proper enlarged space, to which considered processes are transferred, the Frechet symmetry is assured automatically. Namely, in the proper enlarged space, the necessary extremum conditions are obtained by setting to zero the variation of the action integral A based on the Lagrangian $\Lambda = L + \lambda C$ (whichever kinetic potential L and constraints $C=0$ are). These extremum conditions are, of course, the Euler-Lagrange equations of the variational problem for A . With the tool of the Legendre transform, Hamiltonian formulations consistently follow.

Hyperbolic heat transfer, considered in the following sections, is one of examples where the progress resulting from use of the present approach is explicit. Yet the approach can be easily extended to the coupled transfer of heat, mass, and electric charge. With various "gradient or nongradient" rep-

representations of original physical fields in terms of potentials, least action type criteria can be formulated for other processes as well, and corresponding Lagrangian and Hamiltonian formalisms can be developed. Symmetry principles can be considered, and components of the energy-momentum tensor can be evaluated for the accepted kinetic potential L . In each case, an interesting observation follows: the limiting reversible process is a suitable reference frame for analysis of typical irreversible processes.

III. ACTION INTEGRAL AND ADJOINT VARIABLES FOR A DAMPED-WAVE HEAT TRANSFER

We demonstrate here the technique of adjoint representations of physical fields by constructing a variational formulation for the linear process of pure heat conduction (heat flux q) in a rigid solid at rest. The finite speed of propagation of thermal signals is assumed, which means that we decide to use a hyperbolic model rather than parabolic; in particular, the equation of change for the energy density or temperature needs to be a damped-wave equation. All standard equations of change (with parabolic terms) have an absurd physical property: a disturbance (thermal, concentrational, etc.) at any point in the medium is felt instantly at every other point; that is, the velocity of propagation of disturbances is infinite. This paradox is clearly seen in certain routine solutions of parabolic equations; for instance, in the case of heat conduction in a semi-infinite solid on the surface of which the temperature may suddenly increase from, for example, $T=T_0$ to $T=T_s$. The parabolic solution, which is based on the error integral, provides $T=T_0$ for the time $t=0$, but for any very short time $t>0$ and arbitrarily large distances x from the wall one has a $T(x,t)$ different from T_0 in the whole space implying infinitely fast propagation of the disturbance.

The above mentioned nonphysical behavior has been pointed out by many researchers [20–24] and others, and the dilemma was resolved by the acceptance of the hypothesis of heat flux relaxation. The link between the hypothesis and certain results of nonequilibrium statistical mechanics, such as Grad’s solution of the Boltzmann kinetic equation [25], was found [17,26]. The hypothesis is based on the position that Fourier’s law is an approximation to a more exact equation, called the Cattaneo equation, which contains the time derivative of the heat flux along with the flux itself.

For the hyperbolic description of the example considered above, an interesting effect appears for the wall heat flux ($x=0$) when the “driving force is being turned on.” Namely, the wall heat flux, $q(0)$, does not start instantaneously, but rather grows gradually [24] with a rate that depends on a relaxation time τ . After some time the wall heat flux arrives at a maximum and then decreases in time, similar to the Fourier case. This decrease is a classical effect and it occurs since the temperature gradient at the wall decreases in time in the course of heating of our solid. Consequently the Fourier and Fick theories are inappropriate for describing the short-time effects, and although relaxation times are typically very brief (of the order of 10^{-12} s for typical liquids and metals, and 10^{-9} s for gases under normal conditions) the related effects can still have theoretical importance.

Assuming that the heat conduction process is described by the Cattaneo equation of heat transfer and the energy conservation law, the set of constraints is

$$\frac{\partial \mathbf{q}}{c_0^2 \partial t} + \frac{\mathbf{q}}{c_0^2 \tau} + \nabla \rho_e = 0 \quad (1)$$

and

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot \mathbf{q} = 0, \quad (2)$$

where the density of the thermal energy ρ_e satisfies $d\rho_e = \rho C dT$, c_0 is propagation speed for the thermal wave, τ is thermal relaxation time, and the product $D=c_0^2 \tau$ is the thermal diffusivity.

A subtle feature is the irreversible nature of the heat process that requires distinguishing between the trajectories of matter, energy, and entropy. Only in reversible processes entropy or energy “flow with the matter” or they are “linked to the matter,” in irreversible processes the trajectories of entropy or energy differ from those of the matter. Although we restrict ourselves here to a definite coordinate system, the rest frame of the solid, a flow of energy and entropy does occur; the energy flow is represented by the heat flow vector \mathbf{q} . The name “vector \mathbf{q} ” is attributed here to a set of numbers describing the coordinates of \mathbf{q} , as in the matrix theory, without considering any transformation properties of \mathbf{q} to different coordinate frames.

For simplicity we assume the constant values of the fields \mathbf{q} and ρ_e at the boundary. We ignore in this section the vorticity properties of the heat flux, i.e., it is not our concern here whether $\nabla \times \mathbf{q}$ vanishes or is different from zero. Yet we point out that the Cattaneo equation (1) ensures the vanishing rotation for all future times whenever the rotation of the initial field $\mathbf{q}(\mathbf{x},0)$ vanishes. The vorticity properties of the system are discussed in Sec. IV.

For the purpose of a variational formulation, we assume that all dynamical equations of interest constitute “the constraints,” these constraints are adjoined in an action functional A to a singular kinetic potential L that does not contain the derivatives. An important issue that distinguishes the variational formulation considered here from the traditional ones is that one can apply diverse L and always will get a correct variational formulation satisfying the constraints. In fact, there is an infinite number of possible L ’s that can successfully be applied. In particular, for a given vector field \mathbf{u} one can use quadratic L ’s of the structure $L=(1/2)\mathbf{B}:\mathbf{u}\mathbf{u}$, and correct representations of \mathbf{u} can be obtained for any nonsingular quadratic matrix \mathbf{B} . This property, which was first exemplified in an explicit way for a vector set of parabolic equations of change [19] happens because different L ’s yield different representations of physical fields of interest in terms of the Lagrange multipliers of the constraints. These multipliers are, in fact, the potentials of the field; they may be called the Clebsch potentials of the problem, as the well-known Clebsch representations of hydrodynamic velocity use the potential functions that belong to this class. We shall also see that among various L , Hamilton’s structure of L

(designated by L) has a definite preference. We restrict ourselves here to the Lagrangian formalism; yet the results obtained here can be transformed into the Hamiltonian formalism whose main properties for extended thermodynamic systems are described by Grmela and Lebon [27].

An action functional that absorbs constraints (1) and (2) by the Lagrange multipliers, the vector $\boldsymbol{\psi}$ and the scalar ϕ , is taken in the Hamilton's form

$$A = \int_{t_1, V}^{t_2} \varepsilon^{-1} \left\{ \frac{1}{2} \frac{\mathbf{q}^2}{c_0^2} - \frac{1}{2} \rho_e^2 - \frac{1}{2} \varepsilon^2 + \boldsymbol{\psi} \cdot \left(\frac{\partial \mathbf{q}}{c_0^2 \partial t} + \frac{\mathbf{q}}{c_0^2 \tau} + \nabla \rho_e \right) + \varphi \left(\frac{\partial \rho_e}{\partial t} + \nabla \cdot \mathbf{q} \right) \right\} dV dt. \quad (3)$$

In Eq. (3), ε is the energy density at an equilibrium reference state, the constant that ensures the action dimension for A , but otherwise is unimportant. Yet we assume that the actual energy density ρ_e is close to ε , so that the variable ρ_e can be identified with the constant ε in some suitable approximations.

We shall call the multiplier-free term of the integrand (3)

$$L \equiv \frac{1}{2} \varepsilon^{-1} \left\{ \frac{\mathbf{q}^2}{c_0^2} - \rho_e^2 - \varepsilon \right\} \quad (4)$$

the Hamiltonian form of kinetic potential for heat transfer. It is based on the quadratic form of an indefinite sign, and it has usual units of the energy density. It can easily be shown that not far from equilibrium, where ρ_e is close to ε , the two static terms of L yield altogether the density of thermal energy, ρ_e .

This result proves that the limiting structure of L is Hamiltonian, and it should be suitable to describe processes of heat transfer. While, as pointed out in Sec. II, we could use different kinetic potentials, we have shown that the Hamilton's form of L defined by Eq. (4) is the most suitable from the viewpoint of the energy conservation in a limiting reversible process. Thus, in spite of arbitrariness in the accepted L , Hamiltonian structures of the kinetic potential are preferred.

Vanishing variations of action A with respect to multipliers $\boldsymbol{\psi}$ and ϕ recover constraints, whereas those with respect to state variables \mathbf{q} and ρ_e yield representations of state variables in terms of $\boldsymbol{\psi}$ and ϕ . For the accepted Hamilton's structure of L ,

$$\mathbf{q} = \frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \varphi \quad (5)$$

and

$$\rho_e = -\nabla \cdot \boldsymbol{\psi} - \frac{\partial \phi}{\partial t}. \quad (6)$$

In a limiting reversible process (undamped or wave heat conduction for $\tau \rightarrow \infty$) the process is described by purely gradi-

ent representations; the representation for \mathbf{q} then has the structure of the electric field \mathbf{E} expressed in terms of electromagnetic potentials.

For the Hamilton's structure of L , the action A , Eq. (3), in terms of the adjoints $\boldsymbol{\psi}$ and ϕ is

$$A = \int_{t_1, V}^{t_2} \varepsilon^{-1} \left\{ \frac{1}{2c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right)^2 - \frac{1}{2} \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right)^2 - \frac{1}{2} \varepsilon^2 \right\} dV dt. \quad (7)$$

Its Euler-Lagrange equations with respect to $\boldsymbol{\psi}$ and ϕ are, respectively,

$$\frac{\partial}{\partial t} \left\{ \frac{1}{c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right) \right\} + \frac{1}{\tau c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right) - \nabla \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right) = 0 \quad (8)$$

and

$$-\frac{\partial}{\partial t} \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right) + \nabla \cdot \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right) = 0. \quad (9)$$

IV. HYPERBOLIC EQUATIONS FOR ORIGINAL VARIABLES AND THEIR VARIATIONAL ADJOINTS

It is easy to see that Eqs. (8) and (9) are the original equations of the thermal field, Eqs. (1) and (2), in terms of the potentials $\boldsymbol{\psi}$ and ϕ . Their equivalent form below shows the damped-wave nature of the transfer process.

For the Cattaneo equation (1) we obtain from Eq. (8)

$$\frac{\partial^2 \boldsymbol{\psi}}{c_0^2 \partial t^2} - \frac{1}{\tau c_0^2} \frac{\partial \boldsymbol{\psi}}{\partial t} + \frac{\nabla \phi}{\tau} - \nabla (\nabla \cdot \boldsymbol{\psi}) = 0 \quad (10)$$

and, with the energy conservation equation (2), the simplification of Eq. (9) yields

$$-\frac{\partial^2 \phi}{\partial t^2} - \frac{\nabla \cdot \boldsymbol{\psi}}{\tau} + c_0^2 \nabla^2 \phi = 0. \quad (11)$$

Note that the set (10) and (11) becomes decoupled in the reversible case of an infinite τ . Interpreting τ as an average time between the collisions, we can regard the reversible process (with $\tau \rightarrow \infty$) as the collisionless one.

Still another form of heat equations is interesting. While we have obtained Eq. (8) or Eq. (9) as the adjoint representations of the Cattaneo relation (1), a more insightful form is found after one starts with separating the term linear in \mathbf{q} in Eq. (8),

$$-\frac{\partial}{\partial t} \left\{ \frac{1}{c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right) \right\} + \nabla \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right) = \frac{\mathbf{q}}{\tau c_0^2}. \quad (12)$$

Then the ϕ terms of the left-hand side reduce and we are left with

$$-\frac{\partial^2 \boldsymbol{\psi}}{c_0^2 \partial t^2} + \frac{\partial \boldsymbol{\psi}}{\tau c_0^2 \partial t} + \nabla^2 \boldsymbol{\psi} = \frac{\mathbf{q}}{\tau c_0^2}. \quad (13)$$

Thus, for the Cattaneo equation (1), and in terms of the scaled vector potential $\boldsymbol{\Psi}$ such that $\boldsymbol{\Psi} = \boldsymbol{\psi} \tau c_0^2$ the above equation takes the form

$$\nabla^2 \boldsymbol{\Psi} - \frac{\partial^2 \boldsymbol{\Psi}}{c_0^2 \partial t^2} + \frac{\partial \boldsymbol{\Psi}}{\tau c_0^2 \partial t} = \mathbf{q}. \quad (14)$$

For the energy conservation equation (2) we obtain by simplification of Eq. (9),

$$\frac{\partial^2 \phi}{\partial t^2} + \frac{\nabla \cdot \boldsymbol{\psi}}{\tau} - c_0^2 \nabla^2 \phi = 0. \quad (15)$$

Multiplying this equation by τ and eliminating $\boldsymbol{\psi}$ with the help of the energy density representation,

$$\rho_e = -\nabla \cdot \boldsymbol{\psi} - \frac{\partial \phi}{\partial t}, \quad [\text{Eq. (6)}]$$

yields the following equation for the scalar potential:

$$\tau \frac{\partial^2 \phi}{\partial t^2} - \frac{\partial \phi}{\partial t} - \tau c_0^2 \nabla^2 \phi = \rho_e. \quad (16)$$

In terms of the modified scalar potential Φ such that $\Phi = -\phi \tau c_0^2$ (note the minus sign in this definition) the above equation takes the form

$$\nabla^2 \Phi - \frac{\partial^2 \Phi}{c_0^2 \partial t^2} + \frac{\partial \Phi}{\tau c_0^2 \partial t} = \rho_e. \quad (17)$$

Along with the equation (14) for the vector potential, we have thus found the set of four inhomogeneous equations describing dissipative process of heat transfer in terms of the potentials of thermal field, Φ and $\boldsymbol{\Psi}$. They show that the heat flux \mathbf{q} and energy density ρ_e are sources of a thermal field that satisfies the damped-wave equations for the potentials Φ and $\boldsymbol{\Psi}$. The problem of thermal energy transfer is thus broken down to the problem of the related potentials. This is a situation similar to that in electromagnetic theory [28] or in gravitation theory [29], where the specification of sources (electric four current or matter tensor, respectively) defines the behavior of the field potentials. In fact, some equations of heat transfer in terms of these potentials are analogous to inhomogeneous equations for potentials of the electromagnetic field, yet we recognize these analogies as formal only.

The partial differential equations for potentials Φ and $\boldsymbol{\Psi}$ may be contrasted with the differential equations of change for the state variables, ρ_e and \mathbf{q} , which follow from Eqs. (1) and (2). By taking divergence of Eq. (1) and using Eq. (2) we find the telegraphers equation

$$\nabla^2 \rho_e - \frac{\partial^2 \rho_e}{c_0^2 \partial t^2} - \frac{\partial \rho_e}{\tau c_0^2 \partial t} = 0, \quad (18)$$

or its equivalent form, which is the damped-wave equation for the temperature

$$\nabla^2 T - \frac{\partial^2 T}{c_0^2 \partial t^2} - \frac{\partial T}{\tau c_0^2 \partial t} = 0. \quad (19)$$

V. VORTICITY CONSTRAINT AND A GENERALIZED ACTION FUNCTIONAL

A problem arises when we attempt to obtain an equation of the above structure for the heat flux. Indeed, by taking the partial derivative of Eq. (1) with respect to time we conclude that the heat flux density \mathbf{q} satisfies the equation

$$\begin{aligned} \frac{\partial^2 \mathbf{q}}{c_0^2 \partial t^2} + \frac{\partial \mathbf{q}}{\tau c_0^2 \partial t} + \nabla \frac{\partial \rho_e}{\partial t} + \nabla^2 \mathbf{q} &= \frac{\partial^2 \mathbf{q}}{c_0^2 \partial t^2} + \frac{\partial \mathbf{q}}{\tau c_0^2 \partial t} - \nabla(\nabla \cdot \mathbf{q}) \\ &= 0. \end{aligned} \quad (20)$$

With the help of the well-known vector identity

$$\nabla(\nabla \cdot \mathbf{q}) = \nabla^2 \mathbf{q} + \nabla \times (\nabla \times \mathbf{q}) \quad (21)$$

we discover that the heat flux \mathbf{q} satisfies a partial differential equation of the type of telegraphers equations (18) and (19) only if it is irrotational, i.e., if $\nabla \times \mathbf{q} = 0$. We recall that this was an initial assumption of our analysis; it was possible because the Cattaneo equation ensures the vanishing rotation for all future times when the rotation of the initial field $\mathbf{q}(\mathbf{x}, 0)$ vanishes. This observation follows directly from the vorticity form of Eq. (1),

$$\frac{\partial \nabla \times \mathbf{q}(\mathbf{x}, t)}{\partial t} = -\frac{\nabla \times \mathbf{q}(\mathbf{x}, t)}{\tau}, \quad (22)$$

which proves that even if the initial vorticity field is nonvanishing its effect will decay soon because it will relax to zero in accordance with the equation

$$\nabla \times \mathbf{q}(\mathbf{x}, t) = \nabla \times \mathbf{q}(\mathbf{x}, 0) \exp(-t/\tau). \quad (23)$$

Clearly, after a short time, comparable with the average time between collisions, the effects associated with the heat flux vorticity are negligible. Equation (23) also says that the flows \mathbf{q} that are irrotational at the beginning will remain irrotational for any future time t . These conclusions substantiate omission of effects caused by the finite vorticity of heat flux for sufficiently long times. Since, however, the role of the initial vorticity condition may not be ignorable for short times, we stress that there are theoretical tools that allow both to preserve or to ignore vorticity effects. Tools of taking into account the finite vorticity effects are known in the literature of hydrodynamics of adiabatic fluid in the form of the so-called Lin's constraints (Seliger and Whitham [14]), which are build into related action functionals to describe the identity of fluid elements along their Lagrangian trajectories. Yet in problems such as mass diffusion or heat transfer, the identity of the relevant pseudofluid elements does not seem to be at issue in view of the inherent dispersion. If we as-

sume, for example, that the vanishing vorticity is the extra constraint, the action functional is

$$A = \int_{t_1, V} \varepsilon^{-1} \left\{ \frac{1}{2} \frac{\mathbf{q}^2}{c_0^2} - \frac{1}{2} \rho_e^2 - \frac{1}{2} \varepsilon^2 + \boldsymbol{\psi} \cdot \left(\frac{\partial \mathbf{q}}{c_0^2 \partial t} + \frac{\mathbf{q}}{c_0^2 \tau} + \nabla \rho_e \right) - \boldsymbol{\kappa} \cdot \nabla \times \mathbf{q} + \varphi \left(\frac{\partial \rho_e}{\partial t} + \nabla \cdot \mathbf{q} \right) \right\} dV dt. \quad (24)$$

In this functional the vorticity constraint was adjoined to the kinetic potential with the help of the vector potential $\boldsymbol{\kappa}$. The representations of the physical variables in terms of ψ , ϕ , and $\boldsymbol{\kappa}$ are

$$\mathbf{q} = \frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi + \nabla \times \boldsymbol{\kappa} \quad (25)$$

and

$$\rho_e = -\nabla \cdot \boldsymbol{\psi} - \frac{\partial \phi}{\partial t}. \quad [\text{Eq. (6)}]$$

The action A , Eq. (24), expressed in terms of the potentials ψ , $\boldsymbol{\kappa}$, and ϕ is

$$A = \int_{t_1, V} \varepsilon^{-1} \left\{ \frac{1}{2c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi + \nabla \times \boldsymbol{\kappa} \right)^2 - \frac{1}{2} \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right)^2 - \frac{1}{2} \varepsilon^2 \right\} dV dt. \quad (26)$$

Its Euler-Lagrange equations with respect to ψ , ϕ , and $\boldsymbol{\kappa}$ are, respectively,

$$\frac{\partial}{\partial t} \left\{ \frac{1}{c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi + \nabla \times \boldsymbol{\kappa} \right) \right\} + \frac{1}{\tau c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi + \nabla \times \boldsymbol{\kappa} \right) - \nabla \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right) = 0, \quad (27)$$

$$-\frac{\partial}{\partial t} \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right) + \nabla \cdot \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi + \nabla \times \boldsymbol{\kappa} \right) = 0, \quad (28)$$

and

$$\nabla \times \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi + \nabla \times \boldsymbol{\kappa} \right) = 0, \quad (29)$$

where the last equation ensures the vanishing vorticity of heat flux. After separating the terms linear in \mathbf{q} in Eqs. (27) and (28) and rearranging these equations as before we get

$$-\frac{\partial}{\partial t} \left\{ \frac{1}{c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi + \nabla \times \boldsymbol{\kappa} \right) \right\} + \nabla \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right) = \frac{\mathbf{q}}{\tau c_0^2}. \quad (30)$$

Consequently wave equation (14) for $\Psi = \psi \tau c_0^2$ is obtained again

$$\nabla^2 \Psi - \frac{\partial^2 \Psi}{c_0^2 \partial t^2} + \frac{\partial \Psi}{\tau c_0^2 \partial t} = \mathbf{q}. \quad [\text{Eq. (22)}]$$

Moreover, as $\text{div}(\nabla \times \boldsymbol{\kappa}) = 0$, for the energy balance (2) one finds from Eq. (28) the representation (15) again. Hence, as the energy density representation in the form of Eq. (6) is still valid, wave equations (16) or (17) are obtained again for the scalar potentials ϕ and $\Phi = -\phi \tau c_0^2$. Thus, even for generalized actions (24) and (26) we find

$$\nabla^2 \Phi - \frac{\partial^2 \Phi}{c_0^2 \partial t^2} + \frac{\partial \Phi}{\tau c_0^2 \partial t} = \rho_e. \quad [\text{Eq. (17)}]$$

The only difference refers to the vanishing vorticity properties of \mathbf{q} . By taking the partial derivative of Eq. (1) with respect of time and using the vector identity (21) we obtain instead of Eq. (20)

$$\nabla^2 \mathbf{q} - \frac{\partial^2 \mathbf{q}}{c_0^2 \partial t^2} - \frac{\partial \mathbf{q}}{\tau c_0^2 \partial t} = 0 \quad (31)$$

for the irrotational heat flux (29). In this case all basic physical fields, Eqs. (18), (19), and (31), are described by the telegrapher's equations. These are linear PD equations that describe damped heat transfer in solids. Note the difference in sign of linear or "dissipative" terms of these equations in comparison with equations for the potentials. This means that whereas the physical fields are damped due to the (positive) dissipation the potentials are simultaneously amplified due to a "negative dissipation." This also shows how the variational principle deals with non-self-adjoint operators. We may conclude that the Lagrange multiplier approach leads to the potential descriptions much easier and in a more systematic and transparent manner than other approaches.

VI. SOME SPECIAL CASES

An irreversible process constitutes a general case in which both potentials (vector potential $\boldsymbol{\psi}$ and scalar φ) are necessary. To prove this statement let us deal with a simplified action (24) in the single potential but irreversible case of a finite τ . Then a truncated form of general representations (25) and (6) follows. However, the truncated representations are invalid in the case of irreversible processes. In fact, they imply the source term $-\nabla \cdot \boldsymbol{\psi} / \tau = \rho_e / \tau$ for the four divergence of energy, which means the violation of the energy conservation.

The truncated representations are still quite general. In fact, they include the well-known Biot's representations, $\mathbf{q} = \partial \boldsymbol{\psi} / \partial t$ and $\rho_e = \nabla \cdot \boldsymbol{\psi}$, which are the simplest gradient representations of the process (Biot [30]). We thus conclude that from the physical viewpoint Biot's representations should be restricted to reversible processes. They correspond with truncated Cattaneo equation (1) without the irreversible \mathbf{q} term and with a collisionless limit of action (26) when both fields $\boldsymbol{\kappa}$ and φ vanish and only the field ψ is essential. An irrevers-

ible process constitutes a general case in which both potentials (vector potential $\boldsymbol{\psi}$ and scalar φ) are necessary. To prove this statement let us as deal with a simplified action (24) in the single-potential but irreversible case of a finite τ . Then a truncated form of general representations (25) and (6) follows. However, the truncated representations are invalid in the case of irreversible processes. In fact, they imply the source term $-\nabla \cdot \boldsymbol{\psi} / \tau = \rho_e / \tau$ for the four divergence of energy, which means the violation of the energy conservation.

The related reversible action takes in the adjoint space the simplest possible form

$$A = \int_{t_1, V}^{t_2} \varepsilon^{-1} \left\{ \frac{1}{2c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} \right)^2 - \frac{1}{2} (\nabla \cdot \boldsymbol{\psi})^2 - \frac{1}{2} \varepsilon^2 \right\} dV dt. \quad (32)$$

With the simplest (Biot's) representations, or even with their reversible generalizations involving $\boldsymbol{\kappa}$, energy conservation is satisfied identically. Functional (32) then refers to undamped thermal waves that propagate with the speed c_0 and satisfy D'Alembert's equation for the energy density ρ_e or temperature T .

The reversible process is a suitable limiting case to discuss the advantages and disadvantages resulting from the choice of a definite kinetic potential L . As already pointed out, with our choice of L , abandoning the energy conservation constraint in the action (or the formal substitution $\varphi = 0$ in A) is allowed, provided that the Hamiltonian form of the kinetic potential, Eq. (4), is still applied. However, for different L 's the omission of adjoining the energy constraint would not be admissible. For example, a change of the sign of ρ_e^2 in Eq. (4) would result in representations violating energy conservation even in the reversible case, should the Cattaneo equation and the equation of vanishing vorticity of \mathbf{q} be taken as the only adjoined constraints. This substantiates our choice of the Hamiltonian structure of the kinetic potential as the most economical structure. Yet, as already stated, there is considerable flexibility in choosing the kinetic potential when *all* process constraints are adjoined.

VII. ENERGY-MOMENTUM TENSOR AND CONSERVATION LAWS

The energy-momentum tensor is defined as

$$G^{jk} \equiv \sum_i \frac{\partial v_i}{\partial \chi^j} \left[\frac{\partial \Lambda}{\partial (\partial v_i / \partial x^k)} \right] - \delta^{jk} \Lambda, \quad (33)$$

where δ^{jk} is the Kronecker delta and $\chi = (\mathbf{x}, t)$ comprises the spatial coordinates and time. The conservation laws are valid in absence of external fields; they describe then the vanishing four divergences ($\nabla \cdot \partial / \partial \tau$) of G^{jk} . Our approach here follows those of Stephens [13] and Seliger and Whitham [14], where the components of G^{jk} are calculated for Λ gauged by use of divergence theorem along with differentiation by parts. The link of the components of tensor G^{jk} with the partial derivatives of four principal functions S_j , which are solutions of Hamilton-Jacobi equations, is known [31].

Any physical tensor $\mathbf{G} = G^{jk}$ has the following general structure:

$$\mathbf{G} = \begin{bmatrix} \mathbf{T} & -\boldsymbol{\Gamma} \\ \mathbf{Q} & E \end{bmatrix}, \quad (34)$$

where \mathbf{T} is the stress tensor, $\boldsymbol{\Gamma}$ is the momentum density, \mathbf{Q} is the energy flux density, and E is the total energy density.

When external fields are present, the kinetic potential L contains explicitly some of coordinates χ^j . Then the balance equations are satisfied rather than conservation laws,

$$\sum_k \left(\frac{\partial G^{jk}}{\partial x^k} \right) + \frac{\partial \Lambda}{\partial x^j} = 0 \quad (35)$$

for $j, k = 1, 2, \dots, 4$. Equation (35) is the formulation of balance equations for momentum ($j = 1, 2, 3$) and energy ($j = 4$).

We recall the assumption of the small deviation from equilibrium at which our model is physically consistent. With this assumption and for the kinetic potential of Eq. (4) gauged as described above, the gauge action assures that the components of the energy-momentum tensor are multiplier independent. These components are given by Eqs. (36)–(39) below. Respectively, they describe: momentum density Γ^α , stress tensor $T^{\alpha\beta}$, total energy density E , and density of the total energy flux Q^β , which approximately equals q^β .

The momentum density of heat flow follows as

$$\Gamma^\alpha = -G^{\alpha 4} = c_0^{-2} \frac{\rho_e}{\varepsilon} q^\alpha \cong c_0^{-2} q^\alpha, \quad (36)$$

which means that the momentum density for heat is $\Gamma = \mathbf{q} c_0^{-2}$. Whereas, the stress tensor $T^{\alpha\beta}$ has the form

$$G^{\alpha\beta} = T^{\alpha\beta} = \varepsilon^{-1} \left\{ -c_0^{-2} q^\alpha q^\beta + \delta^{\alpha\beta} \left(\frac{1}{2} \mathbf{q}^2 c_0^{-2} - \frac{1}{2} \rho_e^2 + \frac{1}{2} \varepsilon^2 \right) \right\}. \quad (37)$$

This quantity represents stresses caused by the pure heat flow; it vanishes at equilibrium. The total energy density is

$$G^{44} = E^{\text{tot}} = \frac{1}{2} \varepsilon^{-1} c_0^{-2} \mathbf{q}^2 + \frac{1}{2} \varepsilon^{-1} \rho_e^2 + \frac{1}{2} \varepsilon \cong \frac{1}{2} \varepsilon^{-1} c_0^{-2} \mathbf{q}^2 + \rho_e. \quad (38)$$

Finally, we find for the energy flux

$$G^{4\beta} = Q^\beta = \varepsilon^{-1} \rho_e q^\beta \cong q^\beta. \quad (39)$$

In the quasiequilibrium situation ρ_e is very close to ε , then the formal density of the energy flux $G^{4\beta}$ coincides with the heat flux density, \mathbf{q} .

As the heat flux \mathbf{q} is both the process variable and the entity resulting from the variational procedure, the fact that it is recovered here may be regarded as a positive test for the self-consistency of the procedure.

The associated conservation laws for the energy and momentum have the form

$$\frac{\partial (\frac{1}{2} \varepsilon^{-1} c_0^{-2} \mathbf{q}^2 + \rho_e)}{\partial t} = \nabla \cdot (\varepsilon^{-1} \rho_e \mathbf{q}), \quad (40)$$

$$\frac{\partial(c_0^{-2}\varepsilon^{-1}\rho_e q^\alpha)}{\partial t} = \nabla \cdot \left\{ \varepsilon^{-1} \left(-c_0^{-2} q^\alpha q^\beta + \delta^{\alpha\beta} \left(\frac{1}{2} \mathbf{q}^2 c_0^{-2} - \frac{1}{2} \rho_e^2 + \frac{1}{2} \varepsilon^2 \right) \right) \right\}. \quad (41)$$

The energy conservation law (40), which stems from equations (35), (38), and (39), refers to nonequilibrium total energy E that differs from the nonequilibrium internal energy ρ_e by presence of the “kinetic energy of heat” [explicit in our L of Eq. (4) or in Eq. (38)]. The necessity of distinction between E and ρ_e is caused by the property of finite thermal momentum (36) in the frame of stationary skeleton of rigid solid, in which we work. The physical content of results stemming from the quadratic kinetic potential L seems thus acceptable when the system is close to equilibrium. Yet, it should be kept in mind that in this section we evaluated standardized physical components of the matter tensor \mathbf{G} for a given L rather than formal integrals for our model of heat transfer.

VIII. ENTROPY PRODUCTION AND SECOND LAW OF THERMODYNAMICS

Now we evaluate the entropy properties. The entry of \mathbf{G} we need to apply now is $G^{44}=E$ as it is the total energy that is both global and exact conservative property. The density of the conserved energy, E , is a basic variable in the Gibbs relation that links the entropy density ρ_s with E and the current \mathbf{q} . The equality

$$\frac{1}{2} \varepsilon^{-1} c_0^{-2} \mathbf{q}^2 + \rho_e(\rho_s) = E \quad (42)$$

shows that entropy density ρ_s is a function S of E and \mathbf{q} of the following structure:

$$S = \rho_s(\rho_e) = \rho_s \left(E - \frac{1}{2} \varepsilon^{-1} c_0^{-2} \mathbf{q}^2 \right). \quad (43)$$

This means that at the constant mass density the differential of the density S satisfies an extended Gibbs equation,

$$\begin{aligned} dS &= (\partial \rho_s / \partial \rho_e) d \left(E - \frac{1}{2} \varepsilon^{-1} c_0^{-2} \mathbf{q}^2 \right) \\ &= T^{-1} dE - T^{-1} \varepsilon^{-1} c_0^{-2} \mathbf{q} \cdot d\mathbf{q}. \end{aligned} \quad (44)$$

Taking into account that $c_0 = (a/\tau)^{1/2} = [\lambda/(\rho_m C \tau)]^{1/2}$ where λ is the thermal conductivity, one finds $c_0^{-2} = \rho_m C \tau / \lambda = \varepsilon T^1 \tau \lambda^{-1}$ and the above differential can be expressed in terms of λ as

$$dS = T^{-1} dE - T^{-2} \tau \lambda^{-1} \mathbf{q} \cdot d\mathbf{q} \quad (45)$$

Calculating the four-divergence of the entropy flow ($\nabla \cdot \partial / \partial t$) and using the global conservation law for the energy E , Eq. (40), we obtain

$$\begin{aligned} \frac{\partial S}{\partial t} + \nabla \cdot \left(\frac{\mathbf{q}}{T} \right) &= T^{-1} \left(\frac{\partial E}{\partial t} + \nabla \cdot \mathbf{q} \right) - \frac{\tau}{\lambda T^2} \mathbf{q} \cdot d\mathbf{q} + \mathbf{q} \cdot \nabla T^{-1} \\ &= \mathbf{q} \cdot \left(\nabla T^{-1} - \tau T^{-2} \lambda^{-1} \frac{\partial \mathbf{q}}{\partial t} \right) \end{aligned} \quad (46)$$

or in terms equivalent expressions containing λ or c_0 ,

$$\begin{aligned} \frac{\partial S}{\partial t} + \nabla \cdot \left(\frac{\mathbf{q}}{T} \right) &= \mathbf{q} \cdot \left(\nabla T^{-1} - \frac{1}{\varepsilon T c_0^2} \frac{\partial \mathbf{q}}{\partial t} \right) \\ &= \frac{\mathbf{q}}{\lambda T^2} \cdot \left(-\lambda \nabla T - \tau \frac{\partial \mathbf{q}}{\partial t} \right). \end{aligned} \quad (47)$$

But, since Eq. (1) is a simple transformation of the original Cattaneo equation

$$\tau \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -\varepsilon \tau c_0^2 T^{-1} \nabla T = -\lambda \nabla T \quad (48)$$

we arrive at the expression

$$\frac{\partial S}{\partial t} + \nabla \cdot \left(\frac{\mathbf{q}}{T} \right) = \frac{\mathbf{q}^2}{\varepsilon \tau c_0^2 T} = \frac{\mathbf{q}^2}{\lambda T^2}. \quad (49)$$

It describes the second law of thermodynamics in the identically satisfied form, and it holds in both classical irreversible thermodynamics and extended irreversible thermodynamics (EIT, Ref. [32]). Let us recall now that Eq. (48) is as Eq. (1) the result of our variational approach. We have thus obtained confirmation that our approach yields the results in agreement with the second law of thermodynamics. This seems to prove that the accepted kinetic potential whose structure conforms with the Hamilton’s structures encountered in various mechanical action principles has the properties of admissible physical entity to describe the heat flow not far from equilibrium.

As rightly pointed out by some authors [33,34], possessing a kinetic potential that produces only suitable variational equations is by no means sufficient to ascertain that a field theory is sufficient as a whole from the physical viewpoint. This was, in fact, the main reason to test (in Sec. VII and VIII) Noether integrals, conservation laws, and entropy production as consequences of the accepted kinetic potential, Eq. (4). The positive result of these tests [obtained by independent methods and within assumptions of validity of Eqs. (1) and (2)] proves that total energy density, thermal momentum, and all remaining values of the energy-momentum tensor G^{ik} are quantities that are physically admissible in the range of admissibility of linear Cattaneo models (1) and (2). As all these values are relevant to the chosen kinetic potential (4), we can accept this kinetic potential as the entity leading to physical results, with functional expressions in terms of \mathbf{q} and ρ_e described by Eqs. (36)–(49). In effect, from an infinite variety of possible kinetic potentials that can be used in the field description considered (see Sec. II) we accept the sole kinetic potential (4) to reconstitute both the Cattaneo equations and associated extended thermodynamic theory [Eqs. (45)–(49), in agreement with EIT [32]]. It should be underlined that, in view of admissibility of the approximation $\varepsilon^{-1} \rho_e^2 / 2 + \varepsilon / 2 \cong \rho_e$ in Eqs. (4) and (38), the kinetic potential (4) represents—in the framework of the linear theory—the Hamiltonian structure of a difference between part of the energy density related to heat flux (“kinetic energy of heat,” $\varepsilon^{-1} q^2 / 2 c_0^2$) and the density of (nonequilib-

rium) internal energy, ρ_e . Too little is known about nonlinear structures generalizing Cattaneo equation (1) in order to experiment with proposals of a nonlinear theory at the present time. Some of our results for reversible heat flows [17] show that entropy flux $\mathbf{j}_s = \mathbf{q}/T$ may be a better variable than heat flux \mathbf{q} in nonlinear cases. The progress regarding this point will be reported.

IX. GAUGE PROPERTIES OF THERMAL POTENTIALS

The specification of thermal potentials ψ , κ , and ϕ determines unique values of physical fields defined by Eqs. (6) and (25) or any functions of these quantities, such as thermal momentum Γ or total energy E . However, as in case of electromagnetic field, various thermal potentials ψ , κ , and ϕ and kinetic potential L can be attributed to preassigned thermal fields, \mathbf{q} and ρ_e . In cases of this sort it is both natural and standard to determine admissible class of transformed potentials that still ensure unchanged physical fields, and choose from this class definite potentials having the simplest formal structure or certain physical interpretation. In fact, our choice of L , Eq. (4), followed this rule.

Gauging original thermal potentials may lead to those transformed ones that have certain physical interpretations. However, any interpretation of potentials is valid in a particular frame of reference. In the framework of Hamilton's principle for linear and reversible heat transfer, the accepted L , Eq. (4), may be regarded as a quantity that is "already suitably gauged." Biot's interpretation of the thermal displacement vector and his trailing function [30] can be attributed to the potential ψ . Yet, as Eqs. (25) and (6) show, our ψ and ϕ represent altogether the generalization of the Biot's displacement that secures natural treatment of irreversible dynamics and abandons any extraneous concept of a dissipation function added *ad hoc* in the Biot approach. For reversible cases, when ϕ can be gauged to zero, Biot's representation is recovered (Sec. VI). Mathematics of gauging thermal potentials is analyzed below.

As usual in field theories, even if physical fields \mathbf{q} and ρ_e are secured, the fields of Lagrange multipliers ψ , κ , and ϕ are not unique, as the same physical values \mathbf{q} and ρ_e , E , etc., can be represented by various multiplier functions. In general, this change in multipliers can be attributed to changes in kinetic potential L or to transformation of physical constraints in the way ensuring physical equivalence of original and transformed constraints. Gauging thermal potentials is partly similar to that in the theory of electromagnetic field, where the Lagrange multipliers of inhomogeneous Maxwell equations, or the potentials of electromagnetic field (A^0 and \mathbf{A}), are gauged by addition of the partial time derivative of a scalar function to A^0 and subtraction of the gradient of the same function from \mathbf{A} (Jackson [28]). A number of general issues associated with gauge invariant field theories are not discussed here as there are many sources to which the reader can be referred [29,32,35,36]. The significance of gauge groups is also shown in continuum mechanics [37]. When dealing with thermal potentials we focus on the linear thermal model considered rather than on possible nonlinear generalizations.

Let us test the invariance of thermal fields \mathbf{q} , $\nabla \times \mathbf{q}$, and ρ_e and the action functional A when potentials ψ , κ , and ϕ are gauged according to the transformations

$$\psi' = \psi - \nabla \Omega, \quad (50)$$

$$\kappa' = \kappa - \nabla \Omega, \quad (51)$$

and

$$\phi' = \phi + \frac{\partial \Omega}{c_0^2 \partial t} - \frac{\Omega}{c_0^2 \tau}, \quad (52)$$

in which Ω is a gauge scalar function. For transformations (50)–(52) we consider two cases. (1) Ω is completely arbitrary continuous function of \mathbf{x} and t or (2) Ω is the function restricted by the requirement that it should satisfy the following partial differential equation:

$$\frac{\partial^2 \Omega}{c_0^2 \partial t^2} - \frac{1}{c_0^2 \tau} \frac{\partial \Omega}{\partial t} - \nabla^2 \Omega = 0. \quad (53)$$

[The origin of structure of the above restriction and transformation (52) will become clear after considering Eq. (56) below.] After substituting transformations (50) and (51) into field representations of heat flux \mathbf{q} and energy density ρ_e , Eqs. (25) and (6), we find that the heat flux transforms invariantly for arbitrary Ω (meaning that the case 1 occurs), i.e.,

$$\begin{aligned} \mathbf{q}' &= \frac{\partial \psi'}{\partial t} - \frac{\psi'}{\tau} + c_0^2 \nabla \varphi' + \nabla \times \kappa' \\ &= \frac{\partial \psi}{\partial t} - \frac{\psi}{\tau} + c_0^2 \nabla \varphi + \nabla \times \kappa = \mathbf{q}. \end{aligned} \quad (54)$$

Similarly, any definite vorticity of heat flux, $\boldsymbol{\omega} = \nabla \times \mathbf{q}$ (in particular vanishing vorticity $\boldsymbol{\omega} = 0$) satisfies the unconditional gauge invariance

$$\boldsymbol{\omega}' = \nabla \times \kappa' = \nabla \times \kappa = \boldsymbol{\omega}. \quad (55)$$

On the other hand the energy density transforms as

$$\begin{aligned} \rho_e &= -\nabla \cdot \psi' - \frac{\partial \phi'}{\partial t} \\ &= -\nabla \cdot \psi - \frac{\partial \phi}{\partial t} - \frac{\partial^2 \Omega}{c_0^2 \partial t^2} + \frac{1}{c_0^2 \tau} \frac{\partial \Omega}{\partial t} + \nabla^2 \Omega \\ &= \rho_e - \frac{\partial^2 \Omega}{c_0^2 \partial t^2} + \frac{1}{c_0^2 \tau} \frac{\partial \Omega}{\partial t} + \nabla^2 \Omega. \end{aligned} \quad (56)$$

This means that the energy density transforms invariantly only for (restricted) scalars Ω that satisfy the condition (53). Thus the invariance of the whole model of heat transfer refers to the case 2. In other words, the theory assures **both** ρ_e and \mathbf{q} as physical fields provided that condition (53) is satisfied by gauge scalars Ω . Interestingly, the structure of Lorentz condition, well known in the theory of electromagnetic fields (Jackson [28]), appears in the potential representation

of ρ_e . However, in electromagnetic field the *formal* counterpart of our density ρ_e vanishes, i.e., Lorentz gauge condition holds in its classical form, the property that is consistent with the vanishing mass of the photon. In the thermal case considered here, the quantity ρ_e is nonvanishing as it represents the density of the nonequilibrium internal energy. In fact, all analogies we have noted here are weak and formal. They result from the field description accepted in both cases rather than from any serious physical similarities.

Equations (54)–(56) prove that the restricted gauging based on scalars Ω , which satisfy Eq. (53), leaves both fields \mathbf{q} and ρ_e , Eqs. (25) and (6), invariant. In effect, each narrowed gauge transformation (50)–(53) of thermal potentials ψ , κ , and ϕ preserves the same potential representations for \mathbf{q} and ρ_e in the form assuring Cattaneo model of heat transfer, Eqs. (1) and (2). This transformation also ensures invariance of actions A under transformations (50)–(52) in which the scalar Ω satisfied Eq. (53).

X. CONCLUSIONS

This work shows that the problem of thermal energy transfer can be broken down to the problem of related potentials, similar to problems of electromagnetic and gravitational fields. We have found inhomogeneous equations describing dissipative process of heat transfer with a finite propagation speed in terms of thermal potentials, φ and ψ . These equations show that heat flux \mathbf{q} and energy density ρ_e are sources of the field. For heat transfer theory, our results yield a situation similar to that in electromagnetic gravitational field theories, where specification of sources (electric four current or the matter tensor, respectively) defines the behavior of the field potentials. The approach adjoining physical constraints to a kinetic potential by Lagrange multipliers, has thus proven its power and usefulness in the context of quite complicated transfer phenomena in which both reversible and irreversible effects accompany each other. Our analysis proves that thermodynamic irreversibility does not influence the form of the kinetic potential, which remains the Hamiltonian; it only complicates potential representations of physical fields in comparison with those describing reversible evolution. The results show that the heat flux \mathbf{q} has a finite momentum and a related kinetic energy. This is the

energy form that yields inertial properties of heat, and results in the theory satisfying the second law of thermodynamics.

In the variational method developed in Secs. III–VI diverse kinetic potentials L can be applied to produce an infinite number of different, still correct, representations of physical variables \mathbf{q} and ρ_e in terms of field potentials ϕ and ψ . Yet, as shown in Secs. VII and VIII, the physics of the problem of correspondence with Noether's energy and momentum formulas and the satisfaction of second law implies restricting to the kinetic potential (4), which is the Hamiltonian structure in the framework of the linear theory considered. Indeed, in view of the tests in Secs. VII and VIII, the kinetic potential of Eq. (4) may be regarded as a properly gauged L that not only yields the Cattaneo dynamics but also satisfies the above physical requirements. "Nonautonomous" L 's involving time explicitly by an exponential term [38,39] are excluded from considerations as they violate Noether's conservation laws [34]. Comparing with earlier approaches, our method is closer to those of Biot [30] and Lebon [40], as they both work with Biot's thermal potentials that are generalized in our Eqs. (6) and (25).

At the present time too little is known about physics of nonlinear generalizations for Cattaneo equation (1) in order to experiment with proposals of nonlinear theories with variable ρ , c , τ , and λ . Note that, by its own nature, our variational method is relevant to *given* constraints and kinetic potential L . Therefore, in nonlinear generalizations, technical difficulties are on the side of (proper physical generalization of) Cattaneo constraint rather than on that involving the variational method itself. In some nonlinear cases the method can still assure simplicity of potentials ϕ and ψ for a suitably chosen L ; in others, getting explicit potentials is not a trivial task. Some of our earlier results for reversible heat flows [17] seem to imply that entropy flux $\mathbf{j}_s = \mathbf{q}/T$ may be better variable than heat flux \mathbf{q} in nonlinear cases. The progress in this respect will be reported.

ACKNOWLEDGMENTS

This research was supported in part by a grant from the National Science Foundation. One of the authors (S.S.) acknowledges invitation and help from the Chemistry Department of the University of Chicago.

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- [1] R. S. Schechter, *The Variational Method in Engineering* (McGraw-Hill, New York, 1967).
 - [2] S. Sieniutycz, *Conservation Laws in Variational Thermodynamics* (Kluwer Academic, Dordrecht, 1994).
 - [3] F. Vazquez, J. A. del Rio, K. Gambar, and F. Markus, *J. Non-Equilib. Thermodyn.* **21**, 357 (1996).
 - [4] M. M. Vainberg, *Variational Methods for the Study of Nonlinear Operators* (Holden-Day, San Francisco, 1964).
 - [5] B. A. Finlayson, *The Method of Weighted Residuals and Variational Principles* (Academic, New York, 1972).
 - [6] M. Grmela, *Phys. Lett.* **111A**, 36 (1985).
 - [7] M. Grmela and H. C. Ottinger, *Phys. Rev. E* **56**, 6620 (1997); see also, H. C. Ottinger and M. Grmela, *ibid.* **56**, 6633 (1997).
 - [8] A. N. Beris and B. J. Edwards, *Thermodynamics of Flowing Systems With Internal Microstructure* (Oxford University Press, Oxford, 1994).
 - [9] B. Nyiri, *J. Non-Equilib. Thermodyn.* **16**, 39 (1991).
 - [10] F. Markus and K. Gambar, *J. Non-Equilib. Thermodyn.* **16**, 27 (1991).
 - [11] P. Van and B. Nyiri, *Ann. Phys. (Leipzig)* **8**, 331 (1999).
 - [12] J. W. Herivel, *Proc. Cambridge Philos. Soc.* **51**, 344 (1955).
 - [13] J. J. Stephens, *Phys. Fluids* **10**, 76 (1967).
 - [14] R. L. Seliger and G. B. Whitham, *Proc. R. Soc. London, Ser. A* **302**, 1 (1968).
 - [15] R. W. Atherton and G. M. Homsy, *Stud. Appl. Math.* **54**, 31 (1975).

- [16] G. Caviglia, *J. Math. Phys.* **29**, 812 (1988).
- [17] S. Sieniutycz and R. S. Berry, *Phys. Rev. A* **40**, 348 (1989).
- [18] S. Sieniutycz and R. S. Berry, *Phys. Rev. E* **47**, 1765 (1993).
- [19] S. Sieniutycz, *Int. J. Appl. Thermodynamics* **3**, 73 (2000).
- [20] C. Cattaneo, *C. R. Hebd. Seances Acad. Sci.* **247**, 431 (1958).
- [21] P. Vernotte, *C. R. Hebd. Seances Acad. Sci.* **246**, 3154 (1958).
- [22] M. Chester, *Phys. Rev.* **131**, 2013 (1963).
- [23] S. Kaliski, *Bull. Acad. Pol. Sci., Ser. Sci. Tech.* **13**, 211 (1965).
- [24] K. J. Baumeister and T. D. Hamil, *J. Heat Transfer* **91**, 543 (1968).
- [25] H. Grad, in *Handbook der Physik*, edited by S. Flugge (Springer, Berlin, 1958).
- [26] G. Lebon, *Bull. Acad. Soc. Belg. Cl. Sci.* **LXIV**, 456 (1978).
- [27] M. Grmela and G. Lebon, *J. Phys. A* **23**, 3341 (1990).
- [28] J. D. Jackson, *Classical Electrodynamics*, 2nd ed. (Wiley, New York, 1975).
- [29] S. Weinberg, *Gravitation and Cosmology* (Wiley, New York, 1972).
- [30] M. Biot, *Variational Principles in Heat Transfer* (Oxford University Press, Oxford, 1970).
- [31] Y. Guler, *Nuovo Cimento Soc. Ital. Fis., B* **100B**, 251 (1987).
- [32] D. Jou, J. Casas-Vazquez, and G. Lebon, *Extended Irreversible Thermodynamics*, 2nd ed. (Springer, Berlin, 1996).
- [33] D. Balmir and P. Hammond, *Geometry of Electromagnetic Systems* (Oxford University Press, New York, 1996).
- [34] K. H. Anthony, *J. Non-Newtonian Fluid Mech.* **96**, 291 (2001).
- [35] S. Weinberg, *The Quantum Theory of Fields, Vol. I: Foundations* (Cambridge University Press, Cambridge, England 1995).
- [36] D. Gensing and G. Gensing, *Phys. Rev. D* **28**, 286 (1983).
- [37] F. S. Henyey, in *Mathematical Methods in Hydrodynamics and Integrability in Dynamical Systems*, edited by Michael Tabor and Yvain M. Treve, AIP Conf. Proc. No. **88** (AIP, New York, 1982), pp. 85–89.
- [38] B. Vujanovic, *AIAA J.* **9**, 131 (1973).
- [39] B. Vujanovic and S. E. Jones, *Variational Methods in Nonconservative Phenomena* (Academic, New York, 1988).
- [40] G. Lebon, *Quarterly J. Math.* **29**, 499 (1976).