VARIATIONAL PRINCIPLES FOR HEAT CONDUCTION IN DISSIPATIVE CONTINUA

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Applying some results of nonequilibrium statistical mechanics obtained in the framework of Grad's theory we evaluate nonequilibrium corrections Δs to the entropy s of resting incompressible continua in terms of the nonequilibrium density distribution function, f. To find corrections Δe to the energy e or kinetic potential L we apply a relationship that links energy and entropy representations of thermodynamics. We also evaluate the coefficients of the wave model of heat conduction, such as relaxation time, propagation speed, and thermal inertia. With corrections to L we then formulate a quadratic Lagrangian and a variational principle of Hamilton's (least action) type for a fluid with heat flux, or other random-type effect, in the field or Eulerian representation of the fluid motion. Results that are significant in the hydrodynamics of real incompressible fluids at rest and their practical applications are discussed. In particular, we discuss canonical and generalized conservation laws and show the satisfaction of the second law of thermodynamics under the constraint of canonical conservation laws. We also show the significance of thermal inertia and so-called thermal momentum in the variational formulation.

Glossary of symbols

ϕ, Ψ	Lagrange multipliers	p_i	probabilities
Γ	momentum density	P	pressure
ρ_e	energy density	$\boldsymbol{Q}$	energy flux
τ	relaxation time	$\boldsymbol{q}$	heat flux
θ	thermal inertia	R	gas constant
ε	equilibrium energy density	R_j	resistance of jth process
$\mathscr{A}$	action	r_j	rate of jth process
$\boldsymbol{C}$	peculiar velocity	S	total entropy
c_0	propagation speed	$S_v = \rho_s$	entropy density
e	specific energy	s	specific entropy
f	distribution function	T	temperature
G^{jk}	matter tensor	$T^{\alpha\beta}$	stress tensor
g	inertial factor	$\boldsymbol{u}$	macroscopic velocity
H	Hamiltonian	$\boldsymbol{v}$	diffusion velocity
j	flux density	V	potential function
k_B	Boltzmann constant	W	total work

L	kinetic potential	w	specific work
m	mass of microobject	$\boldsymbol{x}$	radius vector
n	particle number	z	Pontryagin's adjoint

1. Introduction

In this research we embed variational principles of heat transfer into the framework of extended thermodynamics and discuss what can be obtained from statistical theories when describing local disequilibria and evaluating kinetic or flux-dependent terms in energies and macroscopic Lagrangians. Assuming an incompressible continuum in the case of fluids we consider them locally at rest, which let us eliminate the effects of hydrodynamic velocity and focus on the heat transfer and the only phenomenon of interest. Sections 2–4 treat statistical aspects of thermodynamic and transport properties of nonequilibrium fluids with heat flow by applying an analysis that uses Grad's results [1958] to determine nonequilibrium corrections Δs or Δe to the energy e or entropy s in terms of the nonequilibrium density distribution function f. To find corrections to the energy e or kinetic potential L we use corrections Δs and a relationship that links energy and entropy representations of thermodynamics. We also evaluate coefficients of the wave model of heat conduction, such as relaxation time, propagation speed and thermal inertial factors, g and θ. With these data we discuss in Sections 5–7 a variational principle of Hamilton's (least action) type for incompressible continua with heat flux in the field or Eulerian representation. We display an approach that adjoins a given set of constraints to a kinetic potential L and transfers the original variational formulation to the space of associated Lagrange multipliers. Also, we evaluate canonical (physical) and formal (Noether's) components of the energy-momentum tensor along with associated conservation laws. We show that despite of the generally noncanonical form of the conservation laws produced by Noether's theorem the approach that adjoins constraints to given kinetic potential works efficiently. In fact, the approach leads to exact embedding of constraints in the potential space of Lagrange multipliers, implying that the appropriateness of the constraining set should be verified by physical rather than mathematical criteria. In fact, the approach is particularly useful in the field (Eulerian) description of transport phenomena, where equations of the thermal field follow from variational principles containing state adjoints rather than original physical variables. An example of the process is hyperbolic heat transfer, but the approach can also be applied to coupled parabolic transfer of heat, mass, and electric charge. With various gradient or nongradient representations of physical fields in terms of state adjoints (quantities similar to those used by Clebsch in his velocity representation [Sieniutycz 1994]), useful action-type criteria emerge. Symmetry principles are effective, and components of the formal energy-momentum tensor can be evaluated. While we focus on heat flow in incompressible continua our work represents, in fact, a quite general approach that shows the methodological advantage of approaches borrowed from the optimal control theory in variational descriptions of irreversible transport phenomena.

2. Information obtained from statistical theories

For irreversible thermodynamic systems statistical theories may be useful [Grad 1958] to evaluate nonequilibrium corrections to energy and other thermodynamic potentials in situations when a continuum is inhomogeneous and this inhomogeneity is associated with presence of irreversible fluxes. To illustrate

benefits resulting from suitable findings in the field of nonequilibrium statistical thermodynamics, heat transfer processes in locally nonequilibrium fluids can be analyzed [Sieniutycz and Berry 1989].

Quite essential in these analyses is the connection between various representations of thermodynamics of nonequilibrium fluids and a relationship that links energy and entropy representations (resembling the Gouy–Stodola law). Thanks to this relationship nonequilibrium corrections to the energy function can be found from those known for the entropy function of Grad's theory. These energy corrections will next be used to construct suitable kinetic potentials L and formulate variational principles.

In this paper we work in the energy and Lagrangian representations of thermodynamics and focus on the formulation of a linear variational description for heat transfer in incompressible continua. While the linearity of the theory is certainly an approximation, it is simple and lucid enough to illustrate the effectiveness of a (relatively unknown) variational approach based on adjoining known process equations as constrains to a kinetic potential which is the integrand of the action functional.

The present approach differs from more conventional variational ones in that the action functional is systematically constructed rather than assumed from the beginning. Once a variational theory is developed for an assumed kinetic potential L it can easily be modified for improved kinetic potentials which take more subtle effects into consideration. Equations of constraints (reversible or irreversible) follow in the form of their representations in the space of Lagrange multipliers as extremum conditions of a composite (constraint involving) Lagrangian Λ or its gauge counterparts. We show that as long as representations describing physical variables of state are known in their explicit form, which expresses these variables in terms of Lagrange multipliers, the whole variational formalism can be transferred to the adjoint space of these multipliers, that is, a variational principle can be formulated in this (adjoint) space. We also show how to use the Lagrangian of the problem to obtain the energy-momentum tensor for the continuum with heat flow and formulate associated conservation laws. Finally we discuss the coincidence conditions for formal and canonical conservation laws.

3. Thermodynamics of heat flow in energy and entropy representations

Here we recall some basic knowledge on the thermodynamics of heat flow without local equilibrium. A process description will be developed that will next be used to construct suitable Lagrangians, variational principles, and conservation laws. We work in the framework of extended thermodynamics of fluids [Jou et al. 2001]. We restrict ourselves to an incompressible, one-component continuum with heat flow. In absence of an external magnetic field the rotation of the system does not change the form of nonequilibrium function $e(s, \rho, \boldsymbol{j}_s)$ which depends then only on the length of the vector $\boldsymbol{j}_s$.

Restricting to second order terms, the following is the McLaurin expansion of e with respect to $\boldsymbol{j}_s = 0$:

$$e(s, \rho, \boldsymbol{j}_s) \cong e(s, \rho, 0) + \tfrac{1}{2}(\partial^2 e/\partial \boldsymbol{j}_s{}^2)_{\rho,s} \boldsymbol{j}_s{}^2, \tag{1}$$

where $e(s, \rho, 0) = e(s, \rho)$ is the familiar equilibrium function of specific energy. Since $(\partial e/\partial j_s)_{\rho,s}$ vanishes at equilibrium, the first-order term is absent in expansion (1), thus the first nonvanishing term is that quadratic with respect to $\boldsymbol{j}_s$. This notion pertains, of course, to any variable vanishing at equilibrium. Clearly, as the second derivative $(\partial^2 e/\partial \boldsymbol{j}_s^2)$ in (1) is determined at constant s and ρ, it depends on these quantities as parameters.

With Equation (1) and for $\boldsymbol{j}_s$ as an independent variable describing nonequilibrium deviations, and not too far from the equilibrium, the following equation for the perfect differential of the specific internal energy e is deduced:

$$de(s, \rho, \boldsymbol{j}_s) = \left[T(s, \rho) + \Delta T(s, \rho, \boldsymbol{j}_s)\right] ds + \left[\rho^{-2} P(s, \rho) + \Delta \rho^{-2} P(s, \rho, \boldsymbol{j}_s)\right] d\rho + \boldsymbol{a}_s(s, \rho, \boldsymbol{j}_s) \cdot d\boldsymbol{j}_s, \quad (2)$$

where $\boldsymbol{a}_s = (\partial^2 e/\partial \boldsymbol{j}_s^2)_{\rho, s} \boldsymbol{j}_s$, from Equation (1). As, roughly, entropy flux $\boldsymbol{j}_s$ is proportional to its momentum density (*thermal momentum* [Sieniutycz and Berry 1989]), the vector quantity $\boldsymbol{a}_s$ is a measure of the associated velocity of entropy diffusion, $\boldsymbol{v} = \boldsymbol{u}_s - \boldsymbol{u}$, where $\boldsymbol{u}_s$ is the absolute velocity of the entropy transfer and $\boldsymbol{u}$ is the hydrodynamic (barycentric) velocity. The latter is, of course zero in the case of the resting fluid we consider. Equation (2) contains corrections ΔT and $\Delta \rho$ which should be added to equilibrium intensities $T(\rho, s)$ and $\rho^{-2} P(\rho, s)$ to obtain proper nonequilibrium values $T(\rho, s, \boldsymbol{j}_s)$ and $\rho^{-2} P(\rho, s, \boldsymbol{j}_s)$. From Equation (2) one obtains the quantities called *nonequilibrium temperatures and pressures*. They are limited in the sense that they are only measures of partial derivatives of the energy with particular nonequilibrium variables chosen to be held constant in a particular frame of variables

$$T(s, \rho, \boldsymbol{j}_s) = \partial e(s, \rho, \boldsymbol{j}_s)_{\rho, j_s}/\partial s \qquad \text{and} \qquad P(s, \rho, \boldsymbol{j}_s) = \rho^2 \partial e(s, \rho, \boldsymbol{j}_s)_{\rho, j_s}/\partial \rho.$$

The last quantity we define is the vector variable $\boldsymbol{a}_s(s, \rho, \boldsymbol{j}_s)$ adjoint with respect to the entropy flux $\boldsymbol{j}_s$ such that

$$\boldsymbol{a}_s(s, \rho, \boldsymbol{j}_s) = \partial \Delta e(s, \rho, \boldsymbol{j}_s)_{\rho, s}/\partial \boldsymbol{j}_s,$$

where $\Delta e = e(s, \rho, \boldsymbol{j}_s) - e(s, \rho, 0)$. We will also use the entropy flux adjoint based on the correction to the energy of unit volume $\Delta \rho_e$

$$\boldsymbol{i}_s(s, \rho, \boldsymbol{j}_s) = \partial \Delta \rho_e(s, \rho, \boldsymbol{j}_s)_{\rho, j_s}/\partial \boldsymbol{j}_s, \quad (3)$$

which has units of momentum per unit entropy and is more important than $\boldsymbol{a}_s$. A discussion on the role of $\boldsymbol{a}_s$ and $\boldsymbol{i}_s$ in the definition of invariant nonequilibrium temperatures is given in Sieniutycz and Berry [1989]. Restricted to the quadratic approximation of Δe in Equation (1) in the case of small flux $\boldsymbol{j}_s$, on the basis of Equations (2), (3), (4) and (5), the nonequilibrium corrections ΔT and ΔP caused by the presence of flux $\boldsymbol{j}_s$ are

$$\Delta T(s, \rho, \boldsymbol{j}_s) = \tfrac{1}{2}\left(\partial^3 \Delta e(s, \rho, \boldsymbol{j}_s)/\partial \boldsymbol{j}_s^2 \partial s\right)_{\text{eq}} \boldsymbol{j}_s^2, \quad (4)$$

with an analogous formula for ΔP. These are quadratic functions of $\boldsymbol{j}_s$. From Equations (1) and (3) the entropy flux adjoint $\boldsymbol{i}_s$ is

$$\boldsymbol{i}_s(s, \rho, \boldsymbol{j}_s) = \left(\partial^2 \rho_e(s, \rho, \boldsymbol{j}_s)/\partial \boldsymbol{j}_s^2\right)_{\text{eq}} \boldsymbol{j}_s. \quad (5)$$

The equilibrium subscript in Equations (4)–(6) means that the corresponding derivatives are evaluated at the limit of $\boldsymbol{j}_s = 0$.

When the curvature of the Gibbs' surface can be neglected, corresponding to the near-equilibrium situation, the energy and entropy excesses are linked by an equality resembling the Gouy–Stodola law

$$(e - e_{\text{eq}})_{s, \rho} = -T(s - s_{\text{eq}})_{e, \rho}. \quad (6)$$

Equation (6) is derived in [Callen 1998, Appendix]. As Figure 1 shows if q is close to zero, an approximation of the same temperature in points A, B, and C can be made. While heat flux densities can be
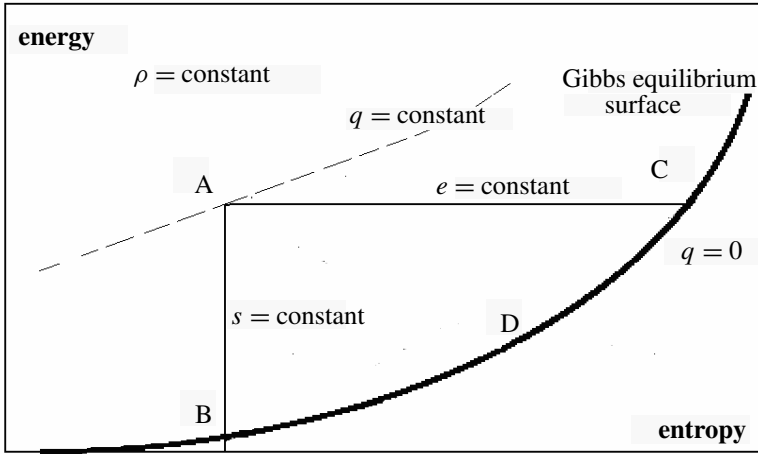
Figure 1. For a given nonequilibrium state, point A, two equilibrium reference states at points B and C correspond, respectively, to the energy and entropy representation. A researcher knowing energy e formulates his description of state A in terms of equilibrium parameters at C for a set of nonequilibrium variables (here heat flux q). However, a researcher who knows entropy s (for example from distribution function f corresponding to A) can base his modeling on the equilibrium properties at B. When point A moves the background, equilibrium states (B and C) vary. The conventional picture of motion in terms of Hamilton's principle corresponds to following the behavior of B and the kinetic energy of entropy flux, whereas the kinetic theory view corresponds to tracking of C and the deviation of entropy from equilibrium. The transition from one view to the other is possible [Sieniutycz and Berry 1989].

finite, they must be small and they are always small otherwise the definition of temperature will lose it meaning. Therefore the small-flux approximation makes sense. Equation (6) is thus interpreted in Figure 1 in the case when the curvature of the line BDC can be neglected and a common temperature T can be attributed to all reference points (B, C, or D) which is allowed for not-too-large distances of point A from equilibrium. The equation states that the energy released during the isoentropic relaxation equals the product of the absolute temperature and the entropy deficiency in the system caused by the presence of an ordered quantity such as the heat flux q or the entropy flux, j_s.

4. Corrections to energy or entropy in terms of nonequilibrium distribution function f

It is the entropy representation that is assumed in the formalism of the kinetic theory of Grad. The function ϕ_1 obtained in Grad's method when the system's disequilibrium is maintained by a heat flux q is

$$\phi_1 = \tfrac{2}{5}\big(m/Pk_B^2T^2\big)\big(\tfrac{1}{2}mC^2 - \tfrac{5}{2}k_BT\big)C \cdot q, \tag{7}$$

where m is the mass of a molecule. Hence one obtains for the entropy deviation

$$\Delta s = -\tfrac{1}{5}(m/\rho Pk_BT^2)q^2. \tag{8}$$

See [Grad 1958; Sieniutycz and Berry 1989; Jou et al. 2001] for more information about Equations (7) and (8). Now Equation (6) is applied to evaluate the related energy deviation in terms of the entropy flux $j_s = qT^{-1}$

$$\Delta e = \tfrac{1}{5}(m^2/k_B\rho^2)j_s^2 = \tfrac{1}{2}\rho^{-2}gj_s^2. \tag{9}$$

Equations (8) and (9) hold to the accuracy of the thirteenth moment of the velocity [Grad 1958]. When passing from Equation (8) to (9) the state equation $P = \rho k_B T m^{-1}$ is used and the constant g of the Taylor expansion of (9) defined as $g(\rho, s) \equiv \rho_{\mathrm{eq}}^2 (\partial^2 e/\partial j_s^2)_{\mathrm{eq}}$ is obtained in the form

$$g \equiv \frac{2mT\rho}{5Pk_B} = \frac{2m^2}{5k_B^2}. \tag{10}$$

Here we have abandoned the entropy representation and use the energy representation.

The knowledge of inertial coefficients, such as g, from statistical mechanics considerations helps calculate two basic quantities in the model of heat transfer in continua with finite wave speed. They are thermal relaxation time τ and the propagation speed, c_0. Of the several formulae available that link quantities τ and g, probably the following expression

$$\tau = kg(\rho T)^{-1} \tag{11}$$

is the most useful [Sieniutycz 1994, p. 199]. Its virtue is that it holds not only for fluids but for arbitrary continua. It links thermal relaxation time τ with thermal conductivity k, inertia g, and thermodynamic state parameters of the system.

As, by definition, the propagation speed of the thermal wave $c_0 = (a/\tau)^{1/2}$, where $a = k/(\rho c_p)$ is the thermal diffusivity, the quantity c_0 satisfies the formula

$$c_0 = \left(\frac{a}{\tau}\right)^{1/2} = \left(\frac{T}{c_p g}\right)^{1/2}.$$

Substituting to this expression the ideal gas data, that is, g of Equation (10) and $c_p = 5k_B/(2m)$, yields the propagation speed in the ideal gas

$$c_0 = \left(\frac{T}{c_p g}\right)^{1/2} = \left(\frac{k_B T}{m}\right)^{1/2}. \tag{12}$$

Thus the results of nonequilibrium statistical mechanics help to estimate numerical values of damped-wave model of heat transfer. The data of τ and c_0 are used below in a variational principle for wave heat transfer. One more coefficient that is quite useful in the wave theory of heat is the coefficient describing a thermal mass per unit of entropy $\theta = Tc_0^{-2}$. For the ideal gas, Equation (12) yields the coefficient $\theta = mk_B^{-1}$. We can now establish a variational principle for linear wave heat flow (Cattaneo model).

5. Adjoining a given set of constraints to a kinetic potential

For a heat conduction process described in the entropy representation by the Cattaneo equation of heat and the conservation law for internal energy, the set of constraints is

$$\frac{\partial q}{c_0^2 \partial t} + \frac{q}{c_0^2 \tau} + \nabla \rho_e = 0 \qquad \text{and} \qquad \frac{\partial \rho_e}{\partial t} + \nabla \cdot q = 0, \tag{13}$$

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

The energy-representation of the Cattaneo equation

$$\frac{\partial \boldsymbol{j}_s}{c_s^2 \partial t} + \frac{\boldsymbol{j}_s}{c_s^2 \tau} + \nabla T = 0 \tag{14}$$

uses diffusive entropy flux $\boldsymbol{j}_s$ instead of heat flux $\boldsymbol{q}$. The coefficient c_s is defined as $c_s \equiv (\rho c_v \theta^{-1})^{1/2}$, where $\theta = T c_0^{-2}$, and thermal diffusivity $k \equiv \rho c_v c_0^2 \tau$. Equation (14) is Kaliski's equation [Sieniutycz 1994]. For an incompressible medium one may apply this equation in the form

$$\frac{\partial \boldsymbol{j}_s}{c_0^2 \partial t} + \frac{\boldsymbol{j}_s}{c_0^2 \tau} + \nabla \rho_s = 0, \tag{15}$$

which uses the entropy density ρ_s a and the propagation speed c_0 instead of c_s.

An action is assumed that absorbs constraints (13) by the Lagrange multipliers, the vector $\boldsymbol{\psi}$ and the scalar ϕ. Its kinetic potential L, Equation (17) below, has a Hamilton's form

$$A = \int_{t_1, V}^{t_2} \varepsilon^{-1} \left\{ \frac{1}{2} \frac{\boldsymbol{q}^2}{c_0^2} - \frac{1}{2} \rho_e^2 - \frac{1}{2} \varepsilon^2 + \boldsymbol{\psi} \cdot \left(\frac{\partial \boldsymbol{q}}{c_0^2 \partial t} + \frac{\boldsymbol{q}}{c_0^2 \tau} + \nabla \rho_e \right) + \phi \left(\frac{\partial \rho_e}{\partial t} + \nabla \cdot \boldsymbol{q} \right) \right\} dV \, dt. \tag{16}$$

Since the continuum is at rest, no kinetic energy appears in the above equation. As the kinetic potentials can be diverse (with accuracy to a four-divergence), the conservation laws for energy and momentum substantiate the form (16). In (16) ε is the energy density at an equilibrium reference state, the constant which ensures the action dimension for A but otherwise is unimportant. 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 suitable approximations.

We call the multiplier-free term of the integrand of Equation (16) the kinetic potential of Hamilton type for heat transfer

$$L \equiv \tfrac{1}{2} \varepsilon^{-1} \left\{ \boldsymbol{q}^2 / c_0^2 - \rho_e^2 - \varepsilon^2 \right\}. \tag{17}$$

It is based on the quadratic form of an indefinite sign, and it has the usual units of the energy density. Remember that we deal with a nonrelativistic theory and in nonrelativistic theories kinetic potentials are always assumed and then tested on their outcomes, never derived. This is what one should remember before he decides to do a variational work. Yet, there may be a hint from Hamilton's principle to define the structure of L in the Hamiltonian form as the difference between the kinetic and static (internal) energy. Functional (17) satisfies this property in the framework of a linear theory that we develop first, because it leads to an explicit analytical solution. It may be shown that Equation (17) is a quadratic approximation of the more exact Hamilton's functional (32) below. This approximation is obtained after the Taylor expansion of the internal energy density around and the subsequent rejection of terms linear in ρ_e which do not influence the extremum conditions of the action integral (16).

Vanishing variations of action A with respect to multipliers $\boldsymbol{\psi}$ and ϕ recover constraints, whereas those with respect to state variables $\boldsymbol{q}$ and ρ_e yield representations of state variables in terms of $\boldsymbol{\psi}$ and ϕ. For the accepted Hamilton-like structure of L, Equation (17), the Euler–Lagrange equations yield

$$q = \frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi$$

and

$$\rho_e = -\nabla \boldsymbol{\psi} - \frac{\partial \phi}{\partial t}. \tag{18}$$

6. Variational formulation in the space of Lagrange multipliers

In terms of the adjoints $\boldsymbol{\psi}$ and ϕ, the action A, Equation (16), assumes the form

$$A = \int\limits_{t_1, V}^{t_2} \varepsilon^{-1} \left\{ \frac{1}{2c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right)^2 - \frac{1}{2} \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right)^2 - \tfrac{1}{2} \varepsilon^2 \right\} dV \, dt. \tag{19}$$

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

$$\frac{\partial}{\partial t} \left\{ \frac{1}{c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right) \right\} + \frac{1}{\tau c_0^2} \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right) - \nabla \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right) = 0 \tag{20}$$

and

$$-\frac{\partial}{\partial t} \left(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t} \right) + \nabla \cdot \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi \right) = 0. \tag{21}$$

It is easy to see that (20) and (21) are the original equations of the thermal field, Equations (13), in terms of the potentials $\boldsymbol{\psi}$ and ϕ. Their equivalent form below shows the damped wave nature of the transfer process. In fact, Lagrange multipliers $\boldsymbol{\psi}$ and ϕ of this (sourceless) problem satisfy certain inhomogeneous wave equations. In terms of the modified quantities $\boldsymbol{\psi}$ and Φ satisfying $\Psi = \psi \tau c_0^2$ and $\Phi = -\phi \tau c_0^2$; these equations are

$$\nabla^2 \boldsymbol{\psi} - \frac{\partial^2 \boldsymbol{\psi}}{c_0^2 \partial t^2} + \frac{\partial \boldsymbol{\psi}}{\tau c_0^2 \partial t} = \boldsymbol{q} \qquad \text{and} \qquad \nabla^2 \Phi - \frac{\partial^2 \Phi}{c_0^2 \partial t^2} + \frac{\partial \Phi}{\tau c_0^2 \partial t} = \rho_e.$$

As both original state variables $(\boldsymbol{q}, \rho_e)$ and adjoints $(\boldsymbol{\psi}, \phi)$ appear in these equations, they represent, in fact, mixed formulations of the theory. Still they are interesting as they show that for given densities $\boldsymbol{q}$ and ρ_e thermal energy transfer can be broken down to potentials. The situation is similar to that in electromagnetic theory or in gravitation theory, where the specification of sources defines the behavior of the field potentials.

Numerical simulation of thermal fields described by (20) and (21) involves the above equations for known potential functions $\boldsymbol{\psi}(\boldsymbol{x}, t)$ and $\phi(\boldsymbol{x}, \tau)$ and given coefficients of wave model, c_0 and τ. The way to calculate the fields $\boldsymbol{\psi}(\boldsymbol{x}, t)$ and $\phi(\boldsymbol{x}, \tau)$ is provided by the variational principle (19). The principle ensures, in fact, optimal values of thermal fields $\boldsymbol{\psi}(\boldsymbol{x}, t)$ and $\phi(\boldsymbol{x}, \tau)$ that are simultaneously solutions of Cattaneo and energy balance equations. In particular, the simulation can involve behavior of imperfect fluids, the application case being polymeric fluids where the quantitative role of relaxation terms is pronounced. Of course, in case of these fluids one should no longer use the ideal gas data but general thermodynamic formulae for coefficients of the wave model, that is, Equation (11), should be applied.

7. Source term in internal energy equation

However, while simple and useful, the method of construction of a suitable action A in the space of potentials by the direct substitution of the representation equations to the kinetic potential L is limited

to cases with linear constraints that do not contain sources. This may be exemplified when the internal energy balance contains a source term $a'\boldsymbol{q}^2$, where a' is a positive constant. The augmented action integral, generalizing Equation (16), should now contain the negative term $-a'\boldsymbol{q}^2$ in its ϕ term

$$-\nabla \cdot \boldsymbol{q} = \frac{\partial \rho_e}{\partial t} - a'\boldsymbol{q}^2. \tag{22}$$

The energy representation is unchanged, but the heat flux representation follows in a generalized form

$$q = (1 - 2a'\phi c_0^2)^{-1}\Big(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi\Big). \tag{23}$$

Substituting Equations (18) and (23) into action A of Equation (16) (L of (17)) shows that in terms of the potentials the action acquires the form

$$A = \int_{t_1, V}^{t_2} \varepsilon^{-1}\bigg\{\frac{1}{2c_0^2}(1 - 2a'\phi c_0^2)^{-2}\Big(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi\Big)^2 - \frac{1}{2}\Big(\nabla.\boldsymbol{\psi} + \frac{\partial \phi}{\partial t}\Big)^2 - \frac{1}{2}\varepsilon^2\bigg\}dV\,dt. \tag{24}$$

However, the Euler–Lagrange equations for this action are not the process constraints in terms of potentials, that is, the method fails to provide a correct variational formulation for constraints with sources. The way to improve the situation is to substitute the obtained representations to a transformed augmented action in which the only terms rejected are total time or space derivatives. The latter can be selected via partial differentiation within the integrand of the original action A. (As we know from the theory of functional extrema the addition of negative terms with total derivatives and divergences do not change extremum properties of a functional.) When this procedure is applied to the considered problem and total derivatives are rejected, a correct action follows in the form

$$A = \int_{t_1, V}^{t_2} \varepsilon^{-1}\bigg\{\frac{1}{2c_0^2}(1 - 2a'\phi c_0^2)^{-1}\Big(\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\boldsymbol{\psi}}{\tau} + c_0^2 \nabla \phi\Big)^2 - \frac{1}{2}\Big(\nabla \cdot \boldsymbol{\psi} + \frac{\partial \phi}{\partial t}\Big)^2 - \frac{1}{2}\varepsilon^2\bigg\}dV\,dt. \tag{25}$$

This form differs from that of Equation (24) only by the power of the term containing the constant a', related to the source. With the related representation equations (18) and (23), action (25) yields the proper Cattaneo constraint (13) (left) and the generalized balance of internal energy which extends (13) (right) by the source term $a'\boldsymbol{q}^2$.

Equation (24) proves that four-dimensional potential space ($\boldsymbol{\psi}, \phi$) is sufficient to accommodate an exact variational formulation for the problem with a source. Yet, due to the presence of this source, the formulation does not exist in the original four-dimensional original space ($\boldsymbol{q}, \rho_e$), and, if somebody insists to exploit this space plus possibly a necessary part of the potential space, the following action is obtained from Equations (18), (23), and (25)

$$A = \int_{t_1, V}^{t_2} \varepsilon^{-1}\Big\{(1 - 2a'\phi c_0^2)\frac{\boldsymbol{q}^2}{2c_0^2} - \frac{1}{2}\rho_e^2 + \frac{1}{2}\varepsilon^2\Big\}dV\,dt. \tag{26}$$

This form of A shows that, when original state space is involved, the state space required to accommodate the variational principle must be enlarged by inclusion of the Lagrange multiplier ϕ as an extra variable. In fact, Equation (26) proves that original state space (physical space) is lacking sufficient symmetry (Vainberg's theorem [Sieniutycz 1994]). Yet, as Equation (26) shows, the adjoint space of

potentials $(\boldsymbol{\psi}, \phi)$, while also four-dimensional as space $(\boldsymbol{q}, \rho_e)$, can accommodate the variational formulation. Why is this so? Because the representation equations do adjust themselves to the extremum requirement of A at given constraints, whereas the given constraints without controls cannot exhibit any flexibility.

Somewhat surprisingly, it follows that a source term in the internal energy balance, as in Equation (22), should be the necessary property of the Cattaneo model, else the energy conservation will be violated. Indeed, aimed at the evaluation of energy conservation we multiply the nontruncated Cattaneo formula

$$\frac{\partial \boldsymbol{q}}{c_0^2 \partial t} + \frac{\boldsymbol{q}}{c_0^2 \tau} + \nabla \rho_e = 0$$

by the heat flux $\boldsymbol{q}$. The result is an equation

$$\frac{\partial \boldsymbol{q}^2}{2\varepsilon c_0^2 \partial t} - \frac{\rho_e}{\varepsilon} \nabla \cdot \boldsymbol{q} + \nabla \cdot (\varepsilon^{-1} \boldsymbol{q} \rho_e) = -\frac{\boldsymbol{q}^2}{\varepsilon c_0^2 \tau}, \tag{27}$$

which describes an energy balance We observe that the combination of this balance with the sourceless balance of internal energy,

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot \boldsymbol{q} = 0,$$

leads to a differential result

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

which — under the linear approximations of the present theory — does not yield a conservation law for the total energy but a balance formula with an energy source

$$\frac{\partial}{\partial t} \left(\frac{\boldsymbol{q}^2}{2\varepsilon c_0^2} + \rho_e \right) + \nabla \cdot (\varepsilon^{-1} \boldsymbol{q} \rho_e) = -\frac{\boldsymbol{q}^2}{\varepsilon c_0^2 \tau}.$$

This shows violation of the total energy conservation for the sourceless internal energy of the model, and leads to the conclusion that the model composed of the Cattaneo equation and sourceless balance of internal energy is physically admissible only in the reversible case of an infinite τ. Certainly, this is not a demanded property of the energy transfer model, thus a further analysis is required. The solution of the dilemma seems to admit a sufficiently large, yet a nonvanishing, source in the internal energy balance.

Admitting a source of the internal energy, as in Equation (22), and using Equation (22) in Equation (27) we find

$$\frac{\partial \boldsymbol{q}^2}{2\varepsilon c_0^2 \partial t} + \frac{\rho_e}{\varepsilon} \frac{\partial \rho_e}{\partial t} - \frac{\rho_e}{\varepsilon} a' \boldsymbol{q}^2 + \nabla \cdot (\varepsilon^{-1} \boldsymbol{q} \rho_e) = -\frac{\boldsymbol{q}^2}{\varepsilon c_0^2 \tau}.$$

From this formula we observe that for a' satisfying

$$a' = \frac{1}{\rho c_0^2 \tau} = \frac{1}{\rho c_v D_h T} = \frac{1}{kT}. \tag{28}$$

and — under the approximation of the linear theory — conservation of total energy is satisfied by the sourceless equation

$$\frac{\partial}{\partial t}\left(\frac{q^2}{2\varepsilon c_0^2} + \rho_e\right) + \nabla \cdot (\varepsilon^{-1} q \rho_e) = 0. \tag{29}$$

The positive value of a' in Equation (28) implies generation of the internal energy in the heat transfer process, as described by Equation (22). Still, the internal energy equation with the positive source caused by the quadratic heat flux is a dubious structure. Nonetheless, it is a step forward in comparison with sourceless internal energy balance as we may observe that this generation awkwardly mimics the entropy production with the coefficient $a = Ta' = 1/k$. This finally leads us to the conclusion that it is the entropy balance with the source j^2/k and that it should replace Equation (22).

Replacing Equation (22) with a' of Equation (28) by its conserved counterpart expressed in entropy terms $T\frac{\partial \rho_s}{\partial t} = -\nabla \cdot q$, where ρ_s is equilibrium entropy density, we expect to obtain better results. After rearranging

$$\frac{\partial \rho_s}{\partial t} = -\nabla \cdot \left(\frac{q}{T}\right) + q \cdot \nabla T^{-1}$$

and using in this result a suitable form of the Cattaneo equation (13) (left)

$$-\frac{\tau}{\lambda T^2}\frac{\partial q}{\partial t} + \nabla T^{-1} - \frac{q}{\lambda T^2} = 0,$$

we obtain

$$\frac{\partial \rho_s}{\partial t} = -\nabla \cdot \left(\frac{q}{T}\right) + q \cdot \left(\frac{\tau}{\lambda T^2}\frac{\partial q}{\partial t} + \frac{q}{\lambda T^2}\right),$$

and hence the second law balance for the entropy of extended thermodynamics is

$$\frac{\partial}{\partial t}\left(\rho_s - \frac{\tau}{2\lambda T^2}q^2\right) + \nabla \cdot (qT^{-1}) = \frac{q^2}{\lambda T^2}.$$

The total energy is conserved in the linearized form (29) or in an exact form

$$\frac{\partial}{\partial t}\left(\frac{T\tau j_s^2}{2k} + \rho_e\right) + \nabla \cdot (T j_s) = 0. \tag{30}$$

We shall now see what can be obtained in the energy representation.

8. Action and extremum conditions in variables j_s and ρ_s

The theory developed so far gives an important hint on how to proceed to a more general formulation which is capable of including the effects of hydrodynamic motion and compressibility of the continuum. Here we shall only outline this problem restricting the variational formulation to the case of resting fluids and relegating all details of the generalized variations to a future paper. In the generalized description we shall proceed to the energy representation, where the constraining set includes Kaliski's counterpart of the Cattaneo equation, Equation (15), and the entropy balance with a source

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho s u + j_s) = a j_s^2. \tag{31}$$

The coefficient a is a positive constant, equal to the reciprocal of thermal conductivity k. The form (31) is valid in both classical and extended thermodynamics. The virtue of using the energy representation is that in this frame there is no need to restrict to the special quadratic form of Equation (17). In fact, here is the proper context to include hydrodynamic effects and to design quite diverse nonlinear expressions of Hamilton's type describing the difference between kinetic and internal energies. Assuming as before the absence of external fields, the kinetic potential L of a general process with hydrodynamic effects follows in the form

$$L = \rho \frac{u^2}{2} + \frac{j_s^2}{2c_s^2} - \rho_e(\rho_s, \rho), \tag{32}$$

where a variable mass density of the fluid is ρ. Equation (32) contains the same kinetic energy of heat which is present in Equation (17), but here this energy is expressed in terms of the entropy flux rather than heat flux. Below we outline the related resting-medium theory.

For a resting medium with a constant density ρ the composite action A assumes the form

$$A = \int_{t_1, V}^{t_2} \left\{ \frac{j_s^2}{2c_s^2} - \rho_e(\rho_s, \rho) + \eta \left(\frac{\partial \rho_s}{\partial t} - a j_s^2 + \nabla \cdot j_s \right) + \psi \cdot \left(\frac{\partial j_s}{c_0^2 \partial t} + \frac{j_s}{c_0^2 \tau} + \nabla \rho_s \right) \right\} dV \, dt. \tag{33}$$

Again, the Lagrange multipliers, scalar η and vector ψ, absorb the process constraints. Equation (33) is a truncated form of a more general action that describes the heat and fluid flow in the case when mass density changes and a finite mass flux (represented by the convection velocity u) is present. This general action is not considered here. The simplified form (33) is sufficient to our present purpose; it selects the heat transfer as the basic process of investigation.

The representations of physical variables in terms of ψ, η and ϕ follow from the stationarity conditions of A. These are

$$\delta j_s : \ (c_s^{-2} - 2a\eta) j_s = \frac{\partial \psi}{c_0^2 \partial t} - \frac{\psi}{c_0^2 \tau} + \nabla \eta, \tag{34}$$

$$\delta \rho_s : \ T(\rho_s, \rho) = -\nabla \cdot \psi - \frac{\partial \eta}{\partial t}. \tag{35}$$

From Equation (34) we obtain a nongradient representation of the diffusive entropy flux in terms of the Lagrange multipliers

$$j_s = (c_s^{-2} - 2a\eta)^{-1} \left(\frac{\partial \psi}{c_0^2 \partial t} - \frac{\psi}{c_0^2 \tau} + \nabla \eta \right). \tag{36}$$

The Lagrange multipliers are potentials in terms of which a variational formulation is constructed. Yet, there is no theoretical argument to assume that the extremum properties of the action applying the above representations in the kinetic potential (32) should generally be the same as those of the augmented quantity (33). The constraint term (with multipliers), while vanishing, also contributes to the extremum properties. What is possible, however, is the partial integration, which ensures that the Euler–Lagrange equations of the augmented and transformed functional are the same. For the functional (33) the partial integration yields the transformed action

$$A' = \int_{t_1, V}^{t_2} \left\{ \frac{j_s^2}{2c_s^2} - \rho_e(\rho_s, \rho) - \rho_s \frac{\partial \eta}{\partial t} - \eta a j_s^2 - j_s \cdot \nabla \eta - j_s \cdot \frac{\partial \psi}{c_0^2 \partial t} + \frac{\psi \cdot j_s}{c_0^2 \tau} - \rho_s \nabla \cdot \psi \right\} dV \, dt. \tag{37}$$

Since the mass density is not varied, we obtain with the representations (35) and (36) a transformed action that includes the free energy density $f_e = \rho_e - T\rho_s$

$$A' = \int_{t_1,V}^{t_2} \left\{ (2a\eta c_s^2 - 1)\frac{j_s^2}{2c_s^2} - (\rho_e - T\rho_s) \right\} dV\,dt. \tag{38}$$

Taking into account that the case of nonvaried mass density corresponds here to the vanishing chemical potential μ, it may be shown that this quantity constitutes a particular type of the pressure action similar to that known in perfect fluid theory. Yet the action obtained includes the Lagrange multiplier η of the entropy balance with the positive source $a\,j_s^2$. The situation is similar to that in the process with a source of internal energy, Equation (25). Namely, to obtain an action functional for an irreversible process of heat transfer, associated with a finite entropy source, the state space required to accommodate the variational principle must be enlarged by inclusion of the Lagrange multiplier η as an extra variable. Yet, in the adjoint space only Lagrange multipliers (potentials) and their derivatives are the arguments of the action integrand. The potential representation of action (38) has the form

$$A' = \int_{t_1,V}^{t_2} \left\{ -\frac{c_s^2}{2(1 - 2a\eta c_s^2)}\left(\frac{\partial \boldsymbol{\psi}}{c_0^2 \partial t} - \frac{\boldsymbol{\psi}}{c_0^2 \tau} + \nabla\eta\right)^2 - f_e\left(-\nabla\cdot\boldsymbol{\psi} - \frac{\partial\eta}{\partial t}, \rho\right) \right\} dV\,dt. \tag{39}$$

Its Euler–Lagrange conditions are Equations (15) and (31) with variables ρ_s and $\boldsymbol{j}_s$ expressed in terms of η and $\boldsymbol{\psi}$, Equations (35) and (36). Thus the variational principle is established.

9. Energy conservation and source term in entropy equation

For Equation (31), the entropy source satisfies $\sigma_s = -\partial L'/\partial\eta$. The total entropy production corresponding to action (39) assures the satisfaction of the second law of thermodynamics

$$S_\sigma = -\frac{\partial A'}{\partial \eta} = \int_{t_1,V}^{t_2} \left\{ \frac{ac_s^4}{(1 - 2a\eta c_s^2)^2}\left(\frac{\partial\boldsymbol{\psi}}{c_0^2 \partial t} - \frac{\boldsymbol{\psi}}{c_0^2 \tau} + \nabla\eta\right)^2 \right\} dV\,dt = \int_{t_1,V}^{t_2} a\,j_s^2 dV\,dt.$$

Let us analyze the differential entropy source in some detail. After transforming the variational stationarity condition of action (37) with respect to $\boldsymbol{\psi}$

$$\frac{\partial\boldsymbol{j}_s}{c_0^2 \partial t} + \frac{\boldsymbol{j}_s}{c_0^2 \tau} + \nabla\rho_s = 0$$

to the form

$$\frac{\partial\boldsymbol{j}_s}{c_0^2 \partial t} + \frac{\boldsymbol{j}_s}{c_0^2 \tau} = -\rho c_v \nabla T^{-1},$$

and using the relation between coefficients c_s and c_0, $c_s^2 = c_0^2(\rho c_v T^{-1})$, we obtain Kaliski's equation of entropy transfer [1965] with the explicit temperature gradient

$$\frac{\partial\boldsymbol{j}_s}{c_s^2 \partial t} + \frac{\boldsymbol{j}_s}{c_s^2 \tau} + \nabla T = 0.$$

After multiplying Kaliski's equation above by $\boldsymbol{j}_s$ we find

$$\frac{\partial\boldsymbol{j}_s^2}{2c_s^2 \partial t} + \nabla\cdot(T\boldsymbol{j}_s) - T\nabla\cdot\boldsymbol{j}_s = -\frac{\boldsymbol{j}_s^2}{c_s^2 \tau}. \tag{40}$$

Under the assumption of the entropy conservation Equation (40) would yield an equation

$$\frac{\partial \boldsymbol{j}_s^2}{2c_s^2 \partial t} + \nabla \cdot (T\boldsymbol{j}_s) + T\frac{\partial \rho_s}{\partial t} = -\frac{\boldsymbol{j}_s^2}{c_s^2 \tau},$$

thus leading to the following energy balance

$$\frac{\partial}{\partial t}\left(\frac{\boldsymbol{j}_s^2}{2c_s^2} + \rho_e\right) + \nabla \cdot (T\boldsymbol{j}_s) = -\frac{\boldsymbol{j}_s^2}{c_s^2 \tau}.$$

This result implies a nonvanishing source of the energy and means that the assumption of the conserved entropy would result in the violation of the energy conservation law.

Yet, for the physical entropy satisfying the nonconserved balance

$$-\nabla \cdot \boldsymbol{j}_s = \frac{\partial \rho_s}{\partial t} - a\boldsymbol{j}_s^2, \tag{41}$$

with the coefficient a equal to the reciprocal of thermal conductivity

$$a = \frac{1}{Tc_s^2 \tau} = \frac{1}{k}. \tag{42}$$

Total energy balance follows from Equations (40)–(42) in a form that is conservative because the two source terms mutually cancel:

$$\frac{\partial}{\partial t}\left(\frac{\boldsymbol{j}_s^2}{2c_s^2} + \rho_e\right) + \nabla \cdot (T\boldsymbol{j}_s) - Ta\boldsymbol{j}_s^2 = -\frac{\boldsymbol{j}_s^2}{c_s^2 \tau}. \tag{43}$$

The action A' that assures the energy conservation is

$$A' = \int_{t_1, V}^{t_2} \left\{ \left(\frac{2\eta - T\tau}{k}\right)\frac{\boldsymbol{j}_s^2}{2} - (\rho_e - T\rho_s) \right\} dV\, dt.$$

Importantly, even when the conservation laws are satisfied in irreversible processes in their canonical form, the related extremum action and potential representations of physical variables do explicitly contain potentials not only their derivatives.

We may thus claim that whenever a irreversible process occurs with the coefficient a satisfying Equation (42), canonical conservation laws can be obtained from Noether's theorem. In particular the energy conservation law has the form

$$\frac{\partial}{\partial t}\left(\frac{\boldsymbol{j}_s^2}{2c_s^2} + \rho_e\right) + \nabla \cdot (T\boldsymbol{j}_s) = 0.$$

As the coefficient $c_s^2 = k(T\tau)^{-1}$, the above equation is equivalent with Equation (30)

$$\frac{\partial}{\partial t}\left(\frac{T\tau \boldsymbol{j}_s^2}{2k} + \rho_e\right) + \nabla \cdot (T\boldsymbol{j}_s) = 0.$$

In conclusion, the mathematical scheme obtained preserves the conservation of energy and simultaneous production of the entropy in accordance with laws of thermodynamics.

10. Concluding remarks

Our statistical evaluation of corrections ΔL to the kinetic potential L has lead to the variational wave model of heat conduction containing relaxation time, propagation speed, and thermal inertia as the basic coefficients. Applying the corresponding action functional and the variational principle of Hamilton's type we have proved generalized conservation laws for energy and momentum which include terms responsible for the effects associated with the heat inertia and obtained the associated second law of thermodynamics. The most important properties of the generalization are a finite momentum of heat and the nonclassical terms in the stress tensor caused by the heat flux. With all this one still has both the first and the second law satisfied. Here the product of temperature T and the positive entropy source of Equation (41) (quadratic in j_s) emerges as the kinetic energy of heat in the energy balance (43). While this result is simple, its role is nontrivial for the existence of the variational formulation. Let us recall that in the variational dynamics of real fluids it is always extremely difficult to simultaneously satisfy both laws of thermodynamics (the classical Hamilton's principle holds only for reversible processes, that is, those without entropy production).

In irreversible situations, it may be necessary to absorb more constraints in the action functional. In fact, thermodynamic irreversibility complicates potential representations of physical fields in comparison with the representations describing the reversible evolution.

The problem of thermal energy transfer can be broken down to the problem of related potentials, as in the case of electromagnetic and gravitational fields. We have displayed inhomogeneous equations describing heat transfer in terms of thermal potentials and sources of the field. These equations show that sources of the thermal field are heat flux q and energy density ρ_e. In heat transfer theory, these results yield a situation similar to that in electromagnetic or gravitational field theories, where specification of sources (electric four-current or the matter tensor, respectively) defines the behavior of the potentials.

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