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Gradient generalization to the extended thermodynamic approach and diffusive-hyperbolic heat conduction

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Abstract

We study a generalization of irreversible thermodynamics with nonlocal closing relation. Thus parabolic and hyperbolic models can be described within one single theory. In the 1-d case, Guyer–Krumhansl equation and classical Fourier heat conduction may be obtained, depending on the constitutive assumptions. The thermodynamical restrictions in form of the Clausius–Duhem inequality are studied taking into account an extra flux of entropy corresponding to nonlocal irreversible effects. Numerical solutions to the resulting initial-boundary value problem are calculated and compared with available experimental results.

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1. Introduction

Propagation of heat waves is a typical low temperature phenomenon which can be observed, for instance, in several dielectric crystals such as Sodium Fluoride (NaF) [1] or Bismuth (Bi) [2]. When a crystal specimen is subjected to the application of a heat impulse at one end, then the impulse results in three output pulses measured at the other hand: a longitudinal and a transversal elastic wave and also a temperature wave, which is called second sound. The speed of propagation of heat pulses has been measured by several authors with a satisfactory precision cf. Refs. [1,2], and suitable fits of experimental data have been obtained in Refs. [3–5]. During the last decade, the increasing interest in nano-technology has opened new perspectives in the analysis of heat transport. Indeed, in micro-devices the mean free path of the heat carriers and the characteristic length of the system become comparable and then the heat transport is no longer diffusive (i.e., determined by the collisions amongst the particles) but ballistic (i.e., determined by the collisions of the particles with the walls). Therefore the classical diffusive heat conduction theory must be generalized in order to take into account such a phenomenology [6–8]. Several models describing nonlinear second sound can be found in the literature [9,10] all yielding the classical Maxwell–Cattaneo–Vernotte equation [11] in the linear case, i.e., when small pulses at a constant and homogeneous background state in a rigid 1-d heat conductor are considered. In the paper [12] we have analyzed the effects of nonlinearity on the solutions of a 4-field model of heat conduction based on the so-called semi-empirical heat conduction theory by Kosiński and co-workers [3,13]. Such a model encompasses the 4-field model of rational extended thermodynamics [10]. We have evaluated the effects of nonlinearity of the governing system of equations on the propagation of heat pulses and found that it has moderate consequences as long as regular solutions of the hyperbolic system are considered.

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In the present paper we want to study the effects of weak nonlocality of the constitutive equations. Weakly nonlocal thermodynamic theories introduce certain space derivatives of the basic variables into the constitutive functions, cf. Ref. [14], hence leading to nonlocal extensions of known continuum theories [15,17].

As far as the evolution of the heat flux is concerned, the most famous nonlocal evolution equation is the celebrated Guyer–Krumhansl equation, which has been derived by solving the linearized Boltzmann equation of phonon gas hydrodynamics [18–20]. It takes the form

$$\dot{q}_i + \frac{1}{\tau_R} q_i = -\frac{1}{3} c_v c^2 \theta_{,i} + \frac{3}{5} c^2 \tau_N (q_{i,jj} + 2q_{k,ki}), \tag{1.1}$$

where i, j, k take the values $1, 2, 3$, θ is the absolute temperature, c_v means the specific heat, τ_R, τ_N and c^2 are material functions whose meaning will be specified in the next section, and q_i denote the components of the heat flux. A superposed dot denotes the time derivative while the subscript $(, k)$ stands for the partial derivative with respect to the cartesian coordinate x_k, $k = 1, 2, 3$. Finally, we have assumed the convention of summation over repeated indices. Let us observe that Eq. (1.1) is linear with respect to the components of the heat flux and their space and time derivatives while the material functions c_v, τ_R, τ_N and c^2 depend on the absolute temperature only. Such an equation can be also obtained in the macroscopic framework of classical irreversible thermodynamics (CIT) [16,17] and extended irreversible thermodynamics (EIT) [21,22]. However, it is not compatible with the mathematical structure of rational extended irreversible thermodynamics (REIT) [23]. In order to explain this statement let us point out the main differences between the REIT, as developed by Müller and Ruggeri [23], and the EIT, proposed by Jou et al. [22]. Both approaches postulate a hierarchical system of balance laws for the evolution of dissipative fluxes, in which the flux at the step n becomes the wanted field at the step $n+1$. However, in EIT the constitutive space can contain also the spacial derivatives of the dissipative fluxes, while in REIT this is not allowed, since, along with the kinetic theory [24,25], the constitutive space is assumed to be rigorously local. On the other hand, it is easily proved that first order nonlocal constitutive equations are sufficient to reproduce the Guyer–Krumhansl behavior [17,21], but these equations are not admitted in the framework of REIT. Hence we face here a paradox, because some results of the kinetic theory cannot be reproduced by REIT due to its particular mathematical structure, which, in turn, follows from the kinetic theory.

In the present paper we propose a gradient extension to the hierarchical system of equations of REIT by allowing the highest order flux of the hierarchical system of equations to depend also on the first spacial derivatives of the wanted fields. This leads to a very general governing equation for the heat flux, from which the Guyer–Krumhansl equation (1.1) can be recovered under some peculiar assumptions on the constitutive functions. On the example of the 1-d rigid heat conductor we shall prove that our generalized 4-field model leads to the Guyer–Krumhansl equation. Numerical solutions to the resulting initial-boundary value problem are calculated as well. These exhibit a smoother behavior than the local 4-field model considered in Ref. [12] due to the presence of a second order spacial derivative in the heat flux equation. With increasing coefficient in front of such a derivative second sound disappears while with decreasing coefficient one reobtains the solutions of the local theory.

For our numerical approach we assign suitable initial and boundary conditions. Although for higher order models the assignment of initial conditions becomes more and more complicated, for the 4-field model it suffices to prescribe the initial temperature and heat flux. At the left boundary we apply Dirichlet conditions (all deviations from equilibrium vanish). At the right boundary we just assume the heat flux to vanish. Such an assumption, together with the semi-discretization, yields an ordinary differential equation for the internal energy at the right boundary.

The paper has the following structure. In Section 2, the generalized 4-field model of REIT is developed on the example of the one-dimensional rigid heat conductor. The compatibility of the constitutive equations with the second law of thermodynamics is investigated by applying the Coleman–Noll procedure [26,27]. However, according to our calculations, in the present case the Liu procedure [28] gives the same results [29].

In Section 3, after proving that the generalized 4-field model yields the Guyer–Krumhansl equation, the material parameters entering the system of equations are identified on the basis of available experimental results.

In Section 4, the numerical method to obtain the solutions to the interesting initial-boundary value problem is illustrated in detail. Then numerical solutions are presented and their properties are discussed.

Finally, in Section 5, concluding remarks together with possible further developments of the theory are presented .

2. Weakly nonlocal thermodynamics of second sound

Let us consider a 1-d rigid heat conductor and let us assume that the evolution of the internal energy and of the heat flux is governed by the 4-field system of REIT [10]

$$\dot{e} + q' = 0, \tag{2.1}$$

$$\dot{p} + N' = -\frac{1}{\tau_R} p. \tag{2.2}$$

We consider the 1-d case only, hence we can abbreviate spacial derivatives simply by prime. Gradient and divergence reduce to the same operation. In Eqs. (2.1)–(2.2) e is the specific internal energy, q is the heat flux, p is the first moment and N the momentum flux.

The name 4-*field theory* comes from the fact that in a 3-d body first order fluxes have three components, so together