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Generalized heat conduction in heat pulse experiments

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ABSTRACT

A novel equation of heat conduction is derived with the help of a generalized entropy current and internal variables. The obtained system of constitutive relations is compatible with the momentum series expansion of the kinetic theory. The well known Fourier, Maxwell–Cattaneo–Vernotte, Guyer–Krumhansl, Jeffreys-type, and Cahn–Hilliard type equations are derived as special cases.

Some remarkable properties of solutions of the general equation are demonstrated with heat pulse initial and boundary conditions. A simple numerical method is developed and its stability is proved. Apparent faster than Fourier pulse propagation is calculated in the over-diffusion regime.

1. Introduction

Recently a common generalization of the Fourier, Maxwell–Cattaneo–Vernotte, Guyer–Krumhansl, Jeffreys-type and Green–Naghdi heat conduction equations was derived in the framework of non-equilibrium thermodynamics [1]. Then experimental and theoretical studies were performed in order to understand the role of different terms and also the possibility of detecting non-Fourier effects [2–4]. According to the basic hypothesis of these investigations, material heterogneities are manifested in additional higher order space and time derivatives in the material functions and result in nonlocal and memory effects (see e.g. [5–7]). However, these effects may be not apparent, the observed phenomena may be Fourier like due to the universal dissipative nature of the additional terms. Therefore it is important to identify and analyze possible qualitative signatures for experimental observation.

The non-equilibrium thermodynamical theory of generalized heat conduction of [1] is based on the assumption of a minimal deviation from local equilibrium. The deviation is expressed in terms of new fields and may appear both in the density and in the current density of the entropy:

– In the entropy a quadratic expression of a vectorial internal variable represents the deviation from local equilibrium in the continua [8,9]. This contribution results in memory effects.
– A generalization of the entropy current density, with the help of current multipliers, represents the deviation of the currents from their local equilibrium form [10–13]. This contribution results in nonlocal effects.

The modifications are restricted only by the second law of thermodynamics, do not incorporate assumptions about the structure of the continua, therefore in this sense the approach is universal [14,15].

An important problematic point of the theory is, that the structure of the derived system of evolution equations seems to be incompatible with the existing theories of Extended Thermodynamics, that is with the hyperbolic system of the momentum series expansion hierarchy of the kinetic theory [16]. In particular it does not compatible with the ballistic phonons, a well explained non-Fourier propagation mechanism in low temperature materials [17,18].

In this paper we slightly modify and extend the approach of [1] introducing the heat flux as a basic field, instead of the general vectorial internal variable of [1]. We also introduce an additional second order tensorial internal variable and the corresponding generalization of the entropy flux by current multipliers. This way we reproduce the first two levels of the hierarchy of kinetic theory in a generalized, phenomenological framework, without any particular assumptions on the structure of the material (e.g. a rarefied gas). We assume only a second law compatible deviation from local equilibrium.

What we obtain is more general than the corresponding set of equations of Extended Thermodynamics, that is the equations obtained from or motivated by the hierarchy of moments in kinetic

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theory. Due to the phenomenological assumptions the whole structure is flexible and we can derive several known generalizations of the Fourier equation in a uniform framework obtaining information regarding their applicability and interrelations. In this respect it is remarkable that Green–Naghdi equations [19–21] are obtained as well as Cahn–Hilliard type heat conduction [22,23]. These heat conduction models were justified by rigorous mathematical methods but not related to Extended Thermodynamics.

Another important property of our approach is that old paradoxes and reservations regarding some forms of heat conduction are shown in a new light. For example the well discussed paradox of heat waves with negative values of temperature of the Maxwell–Cattaneo–Vernotte and the Jeffreys-type equations (see e.g. in [24,25]) seems to be removed simply because thermodynamics requires the gradient of the reciprocal temperature instead of the gradient of the temperature in the related terms of the equations.

This paper focuses on the problem of observability of non-Fourier heat conduction from a theoretical point of view. Solving generalized heat conduction models with heat pulse initial and boundary conditions will demonstrate that Fourier type solutions may appear unexpectedly and therefore in addition of wavelike effects one may look for other observable benchmarks of heat conduction beyond Fourier.

In the next section we introduce the theory and derive the heat conduction equation up to the second current multiplier and show some known particular cases. The third section describes the heat pulse experiment, then we introduce a simple finite difference numerical method to solve the set of equations. Finally, in the fifth section, we show some demonstrative solutions of the equations on the example of laser flash experiment in order to identify possible non-Fourier effects.

2. Non-equilibrium thermodynamics of heat conduction

In this paper we restrict ourselves to rigid heat conductors, therefore the time derivatives are partial and the density of the material is constant. Our starting point is the balance of internal energy:

$$\partial_t e + \nabla \cdot \mathbf{q} = 0. \tag{1}$$

Here e is the density of the internal energy, and $\mathbf{q}$ is the heat flux, the current density of the internal energy. ∂_t denotes the partial time derivative and ∇ with the central dot is the divergence, $\nabla \cdot \mathbf{q} = tr(\nabla \mathbf{q})$.

The second law is given in the following form

$$\partial_t s + \nabla \cdot \mathbf{J} \geqslant 0. \tag{2}$$

Here s is the entropy density and $\mathbf{J}$ is the entropy current density vector. For modeling phenomena beyond local equilibrium, we introduce the heat flux $\mathbf{q}$ as basic field variable and also a second order tensorial internal variable denoted by $\mathbf{Q}$. The advantage of using the heat flux as basic field quantity instead of a vectorial internal variable of the treatment in [1] is the easier comparison with Extended Thermodynamics. The deviation from local equilibrium will be characterized by two basic constitutive hypotheses:

– We assume a quadratic dependence of the entropy density on the additional fields [8]:

$$s(e, \mathbf{q}, \mathbf{Q}) = s_{eq}(e) - \frac{m_1}{2}\mathbf{q} \cdot \mathbf{q} - \frac{m_2}{2}\mathbf{Q} : \mathbf{Q}, \tag{3}$$

where m_1 and m_2 are positive constant material coefficients. This is not a complete isotropic representation, for the sake of simplicity we have introduced a single material coefficient for the second order tensor $\mathbf{Q}$, too. The derivative of the local equilibrium part of the entropy function s_{eq} by the internal energy is the reciprocal temperature: $\frac{ds_{eq}}{de} = \frac{1}{T}$ and $\mathbf{Q} : \mathbf{Q} = tr(\mathbf{Q} \cdot \mathbf{Q})$. The quadratic form may be considered as a first approximation in case of the heat flux and is due to the Morse lemma for the internal variable [9]. The sign is determined requiring concave entropy function, that is, thermodynamic stability [18,17].

– We assume that the entropy flux is zero if $\mathbf{q} = 0$ and $\mathbf{Q} = 0$. Therefore it can be written in the following form:

$$\mathbf{J} = \mathbf{b} \cdot \mathbf{q} + \mathbf{B} : \mathbf{Q}. \tag{4}$$

Here $\mathbf{b}$ is a second order tensorial constitutive function and $\mathbf{B}$ is a third order one. They are the current multipliers introduced by Nyíri [11]. General aspects of this assumption were treated in [12] and the special case of heat conduction was considered in [1,6].

Now the basic fields are $T, \mathbf{q}$ and $\mathbf{Q}$, the constitutive functions are $\mathbf{b}$ and $\mathbf{B}$. The entropy production is:

$$\begin{aligned}\partial_t s + \nabla \cdot \mathbf{J} &= -\frac{1}{T}\nabla \cdot \mathbf{q} - m_1 \mathbf{q} \cdot \partial_t \mathbf{q} - m_2 \mathbf{Q} : \partial_t \mathbf{Q} + \mathbf{b} : \nabla \mathbf{q} + \mathbf{q} \cdot (\nabla \cdot \mathbf{b}) \\ &\quad + \mathbf{B} \,\vdots\, \nabla \mathbf{Q} + \mathbf{Q} : (\nabla \cdot \mathbf{B}) = \left(\mathbf{b} - \frac{1}{T}\mathbf{I}\right) : \nabla \mathbf{q} + (\nabla \cdot \mathbf{b} - m_1 \partial_t \mathbf{q}) \cdot \mathbf{q} \\ &\quad + (\nabla \cdot \mathbf{B} - m_2 \partial_t \mathbf{Q}) : \mathbf{Q} + \mathbf{B} \,\vdots\, \nabla \mathbf{Q} \geqslant 0.\end{aligned} \tag{5}$$

Here $\mathbf{I}$ is the unit tensor and the triple dot denotes the full contraction of third order tensors. In the last two rows the first and the third terms are products of second order tensors, the second term is the product of vectors and the last term is of third order ones. The time derivatives of the state variables $\mathbf{q}$ and $\mathbf{Q}$ represent their evolution equations, here they are constitutive quantities. Therefore one can identify four thermodynamic forces and currents in the above expression and assume linear relationship between them in order to obtain the solution of the entropy inequality.

The third and fourth force–current pairs are related to the tensorial internal variable $\mathbf{Q}$. In case of isotropic materials only the second order tensors can show cross effects (extended thermal and internal interactions), the vectorial (thermal) and third order tensorial terms (extended internal) are independent (see Table 1).

In the following we will simplify the treatment and develop the theory in one spatial direction. In the one dimensional representation of the tensors we remove the boldface letters, and the one dimensional spatial derivative is denoted by ∂_x.

In this case the entropy production can be rewritten as:

$$\left(b - \frac{1}{T}\right) : \partial_x q + (\partial_x b - m_1 \partial_t q)q + (\partial_x B - m_2 \partial_t Q)Q + B\partial_x Q \geqslant 0. \tag{6}$$

The linear relations between the thermodynamic fluxes and forces result in the following constitutive equations:

$$m_1 \partial_t q - \partial_x b = -l_1 q, \tag{7}$$

$$m_2 \partial_t Q - \partial_x B = -k_1 Q + k_{12} \partial_x q, \tag{8}$$

$$b - \frac{1}{T} = -k_{21} Q + k_2 \partial_x q, \tag{9}$$

$$B = n \partial_x Q. \tag{10}$$

The entropy inequality (6) requires the following inequalities

$$l_1 \geqslant 0, \;\; k_1 \geqslant 0, \;\; k_2 \geqslant 0, \;\; n \geqslant 0, \;\; \text{and} \;\; K = k_1 k_2 - k_{12} k_{21} \geqslant 0. \tag{11}$$

The above set of constitutive Eqs. (7)–(10) together with the energy balance (1) and the caloric equation of state $T(e)$ give a solvable set of equations, with suitable boundary and initial conditions. In case of constant coefficients one can easily eliminate the current multipliers by substituting them from Eqs. (9) and (10) into Eqs. (7) and (8) and obtain: