



Dynamical temperature and generalized heat-conduction equation



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ABSTRACT

By means of a dynamical non-equilibrium temperature we derive a generalized heat-conduction equation which accounts for non-local, non-linear, and relaxation effects. The dynamical temperature is also capable to reproduce several enhanced heat equations recently proposed in literature. The heat flux is supposed to be proportional to the gradient of the dynamical temperature, and the material functions are allowed to depend on temperature. It is also pointed out that the heat flux cannot assume arbitrary values, but it is limited from above by a maximum value which ensures that the thermal conductivity remains positive.

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1. Introduction

In Classical Irreversible Thermodynamics (CIT) [1] the Fourier law

$$q_i = -\kappa\theta_{,i}, \quad (1)$$

relates the heat flux q_i both to the gradient of the thermodynamic non-equilibrium temperature θ and to the temperature-dependent thermal conductivity κ . Second law of Thermodynamics forces the thermal conductivity to be a positive-definite function.

For rigid bodies, the combination of Eq. (1) with the local balance of the energy in the absence of heat supply

$$\rho\dot{u} + q_{i,i} = 0, \quad (2)$$

with ρ as the mass density and u as the specific internal energy, provides the evolution equation for the temperature, once u is expressed as a function of θ by a constitutive equation.

The use of Eq. (1) allows a satisfactory description of heat conduction in several situations at the macroscopic length scale, but it is unable to describe accurately the same phenomenon at nanoscale. In fact, whenever crystalline solids are confined to the nanometer range, heat transport within them is strongly altered by several phenomena as, for example, the phonon quantization, changes in phonon dispersion relation, increased boundary scattering, etc. The behavior of nanodevices is also influenced by non-linear effects, which lack in the Fourier law. Furthermore, in micro-

nano-devices working at high frequencies, the heat flux has no enough time to accommodate to the value given by the Fourier law, so that one has also to take into account the relaxation time of the heat flux [2–4]. As a consequence, several new heat-transport theories appeared in literature in the last three decades. Many of them have been analyzed in Ref. [5], wherein their connection with different approaches to non-equilibrium thermodynamics has been pointed out. Here we pursue the previous analysis by considering the thermomass (TM) theory [6–11], i.e., a recent heat-conduction theory which in rigid bodies regards the heat as transported by a gas-like collection flowing through the crystal lattice.

In the present paper we derive by proper thermodynamical methods a generalized heat-transport equation, primarily focusing our attention on the concept of non-equilibrium temperature. The correct definition of temperature at nanoscale is, in fact, a further interesting and not yet explored problem [12–14]. The usual definition of temperature, related to the average energy of a system of particles, is valid for systems in (or very close to) equilibrium, when the time derivative of the average energy is negligible. Once the interest lays in the transport of heat through a nanosystem, instead, one has to keep in mind that the system is in very strong non-equilibrium situations.

In Refs. [15–19] both classical and enhanced heat-transport equations have been obtained by means of a dynamical temperature β which principally differs from θ by a frictional term which is responsible of the finite speed of propagation of thermal disturbances. The main differences between β , θ and the local-equilibrium temperature T are carried out in Ref. [18]. Note further, that according to the terminology of CIT [1,20,21], β can be also regarded as an internal state variable [22–24].

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The dynamical temperature has its own evolution equation which, in the very general case, reads

$$\dot{\beta} = f(\Sigma), \tag{3}$$

where f is a regular function defined on the state space Σ . For instance, if θ and β enter the state space, Eq. (3) can be written as

$$\dot{\beta} = \frac{F(\theta, \beta)}{\tau_R}, \tag{4}$$

with F a suitable smooth function, and τ_R a temperature-dependent relaxation time related to resistive processes of interaction among the heat carriers, and the order of magnitude of which is in the interval $[10^{-12} \text{ s}; 10^{-9} \text{ s}]$ in the case of second-sound propagation at low temperature [5]. The conditions

$$\frac{\partial F}{\partial \theta} \geq 0, \quad \frac{\partial F}{\partial \beta} \leq 0, \tag{5}$$

ensure, respectively, that:

1. in thermodynamic equilibrium, with θ equal to T [13,25], β is a regular function of T and the order relation \leq between different temperatures is preserved;
2. the solutions of Eq. (4) are stable.

In the simplest case the previous conditions are realized by the following linear evolution equation:

$$\dot{\beta} = -\frac{\beta - \theta}{\tau_R}, \tag{6}$$

which will be generalized in Section 2 in order to take into account non-local effects.

In Refs. [15,16,18] it is postulated that the heat flux is proportional to the gradient of β by means of the following Fourier-type heat-conduction law:

$$q_i = -\lambda \beta_{,i}, \tag{7}$$

where λ denotes the thermal conductivity expressed as a function of the specific internal energy. The one-to-one relation between θ and u allows to set a strict relation between the thermal conductivity κ in Eq. (1) and the thermal conductivity λ in Eq. (7), namely, we have $\lambda(u) \equiv \kappa(\theta(u))$. From the positivity of $\kappa(\theta)$, it follows that the function $\lambda(u)$ is positive definite, too.

Once the evolution equation for β has been derived, different heat-transport regimes can be described. For instance, whenever the material functions τ_R and λ can be considered constant (for example, when they only show slight changes with the temperature), the combination of Eqs. (7) and (6) leads to the well-known Maxwell–Cattaneo equation [18,19]

$$\tau_R \dot{q}_i + q_i = -\lambda \theta_{,i}, \tag{8}$$

which provides a satisfactory description of high-frequency thermal waves. Although Eq. (8) is capable to describe relaxation effects, it does not account for non-linear effects, which may enter the heat-transport equation both as a temperature dependence in the material functions, and as the presence of non-linear products of the temperature gradient (or of the heat flux). These effects, instead, will be described by our generalized heat equation.

The paper runs as follows.

In Section 2, we develop the aforementioned model by establishing the state space and the evolution equations characterizing the system at hand. Moreover, we exploit the entropy principle in order to obtain necessary and sufficient conditions ensuring the compatibility of the model with second law of thermodynamics [1].

In Section 3, we provide a solution of the system of thermodynamic restrictions found in Section 2, proving so that the model is physically admissible.

In Section 4, we derive a generalized heat-conduction equation accounting for non-linear and relaxation effects.

In Section 5 we show that our generalized heat-conduction equation encompasses the heat-conduction equation of the thermomass theory [6–11].

Finally, in Section 6, we discuss the main results through the prism of the concept of non-equilibrium temperature. After observing that the heat flux cannot assume arbitrary values, but it is limited from above by a maximum value which ensures that the thermal conductivity remains positive, we show that such a limit value is determined by the thermodynamic absolute temperature as well as by the dynamical one.

2. Nonlinear gradient-dependent transport law

In this section we postulate a suitable evolution equation for β and analyze its compatibility with second law of thermodynamics [1].

Before to proceed in this analysis, let us observe that the considerations of previous section suggest that in an equilibrium system, where the specific internal energy u is a function of the thermodynamic local-equilibrium absolute temperature T , the use of both u and β would be redundant. However, out of equilibrium, where u does not display the same distribution as in equilibrium, β is a truly independent quantity, not redundant with u . Thus, we are allowed to consider a rigid heat conductor at rest, characterized by the following state space:

$$\Sigma = \{u; \beta; \beta_{,i}\},$$

where, in view of Eq. (7), the further state variable $\beta_{,i}$ means that the heat flux enters the state space. This is in accordance with the basic tenets of Extended Irreversible Thermodynamics (EIT), a recent thermodynamic theory in which includes the dissipative fluxes in the set of the independent thermodynamic variables [1,12,26].

Then, an evolution equation for β of the form (3) can be postulated. Here we suppose that

$$\dot{\beta} = \frac{u}{\sigma} - \frac{\beta}{\tau} + \frac{A}{2} \beta_{,i} \beta_{,i}, \tag{9}$$

wherein σ , τ and A are regular scalar functions of u . Eq. (9), besides accounting for the possible variations of the different thermophysical quantities with respect to the temperature, enhances Eq. (6) by extending the evolution of β in the realm of weakly non-local thermodynamics. Hence, if for example, one assumes $\tau(u) = \tau_R(\theta)$ and $\sigma \equiv c_v \tau_R$ with c_v being the specific heat at constant volume, then Eq. (9) becomes

$$\dot{\beta} = -\frac{(\beta - \theta)}{\tau_R} + \frac{A}{2} \beta_{,i} \beta_{,i}, \tag{10}$$

which is indeed physically superior to Eq. (6) since, according to Eq. (6) β reduces to θ in non-equilibrium steady states, whereas if Eq. (10) holds, in steady states θ and β are still related by a partial differential equation. Thus, Eq. (9) (or, equivalently, Eq. (10)) describes not only the usual aspect of β dependent explicitly on time, but also a new aspect dependent on its gradient. This feature is related to the fact that in the presence of a gradient the system is locally receiving an energy input and it is yielding an energy output to the nearby regions. This implies a dynamical aspect even in the steady states, where energy input rate is equal to the energy output rate.

By means of the constitutive equation (7), Eq. (2) can be rewritten as

$$\rho \dot{u} - \beta_{,k} u_{,k} \frac{\partial \lambda}{\partial u} - \lambda \beta_{,ik} \delta_{ik} = 0, \tag{11}$$

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