



M. Di Domenico · A. Sellitto · V. Zampoli

Thermal pulse propagation beyond the Maxwell–Cattaneo theory: Application to one-dimensional nanosystems

Received: 18 April 2022 / Accepted: 22 July 2022 / Published online: 11 August 2022
© The Author(s) 2022

Abstract A non-local and non-linear thermodynamical model of heat transfer at nanoscale beyond the well-known Maxwell–Cattaneo theory is derived. The compatibility of the proposed model with second law of thermodynamics is proved. The model is subsequently used to investigate the propagation of a heat pulse in one-dimensional nanosystems in the linear case. The predicted results are compared with those arising from the Maxwell–Cattaneo theory in order to point out the possible influence both of the non-local effects, and of the relaxation effects of the higher-order fluxes. Some problems related to initial data and boundary conditions are also discussed.

Keywords Hyperbolic heat transfer · Pulse propagation · Second sound · Wave front · Memory effects · Non-local effects · Non-linear effects · Laplace transform

1 Introduction

In the general context of continuum mechanics, a very important role is played by the so-called balance laws. From the theoretical point of view, a balance law is just the statement of the causes of the contents time-changes of a certain extensive physical quantity over a given domain. Those causes can be only of the following two different types:

- (i) Flux. The physical quantity varies owing to possible exchanges with the surroundings through the boundary of the domain.
- (ii) Production. The physical quantity varies since some (thermodynamic) process may occur inside the domain.

From the practical point of view, each balance law is expressed in terms of a partial differential equation (i.e., the so-called balance equation) which is usually written in a local form in such a way that it has to be valid in any point of a given domain. Among the different balance equations, in non-equilibrium thermodynamics

Communicated by Andreas Öchsner.

M. Di Domenico · A. Sellitto
Department of Industrial Engineering, University of Salerno, 84084 Fisciano, Italy
E-mail: madidomenico@unisa.it

A. Sellitto
E-mail: ant.sellitto@gmail.com

V. Zampoli (✉)
Department of Information and Electrical Engineering and Applied Mathematics, University of Salerno, 84084 Fisciano, Italy
E-mail: vzampoli@unisa.it

a great importance deserves the (local) balance equation of the specific entropy s (per unit volume), namely,

$$\partial_t s = -J_{i,i}^{(s)} + \sigma^{(s)} \quad (1)$$

with $J_i^{(s)}$ being the specific-entropy flux, and $\sigma^{(s)}$ the specific-entropy production (per unit volume). In Eq. (1) the term $J_{i,i}^{(s)}$ (which accounts for the rate of local-entropy exchanged with the surroundings) may be zero, positive, or negative; according to the second law of thermodynamics, instead, in Eq. (1) the quantity $\sigma^{(s)}$ (deriving from processes occurring inside the system) has to be always non-negative (namely, it is zero at equilibrium, or for reversible transformations, whereas it is larger than zero for irreversible transformations) in any point and at any time, whatever the thermodynamic process is [1,2]. Since $\sigma^{(s)}$ points out the sources of irreversibility occurring in any thermodynamic process, it should be (directly, or indirectly) related to all quantities which characterize the irreversible process at hand. In non-equilibrium thermodynamic theories, in fact, the physical constraint

$$\sigma^{(s)} \geq 0 \quad (2)$$

plays a very important role: since all solutions of the balance equations have to comply with the condition in Eq. (2), in those theories that unilateral constraint is mainly used to determine the forms either of the constitutive relations [3], or of the evolution equations of the state-space variables [2]. In pursuing these goals, as it will be briefly shown below in the case of two very well-known theories of heat transfer in a rigid body (just for the sake of simplicity), besides the correct choice of the state-space variables, a crucial point is also the right setting of the relation between the specific-entropy flux $J_i^{(s)}$ and the local heat flux q_i [4-6].

1.1 The Fourier theory

In the case of the Fourier (F-) theory of the heat transfer in a rigid body, the specific internal energy (per unit volume) u is the only state-space variable: in the F-theory, therefore, only the evolution equation of u is needed. The time variations of u , indeed, are stated by the balance law of energy, the local formulation of which reads

$$\partial_t u = -q_{i,i}. \quad (3)$$

According to the point of view of the balance law, as a consequence, from Eq. (3) one may straightforwardly note that q_i is just the flux of u : the heat flux, therefore, is the only cause of time variations of the internal energy, in the absence of a source term (here and in what follows neglected just for the sake of simplicity). Since in this theory $s = s(u)$, moreover, the use of Eq. (3) yields

$$\partial_t s \equiv \left(\frac{ds}{du} \right) \partial_t u = -\frac{q_{i,i}}{\theta} \quad (4)$$

once the usual relation

$$\frac{ds}{du} = \frac{1}{\theta} \quad (5)$$

is employed,¹ with θ being the non-equilibrium temperature [2,7,8]. If we recall that the classical constitutive assumption for the entropy flux states that the specific-entropy flux only depends on the heat flux and the non-equilibrium temperature [1], i.e.,

$$J_i^{(s)} = \frac{q_i}{\theta} \quad (6)$$

then Eq. (4) can be also rewritten as

$$\partial_t s = -J_{i,i}^{(s)} - \left(\frac{q_i}{\theta^2} \right) \theta_{,i}. \quad (7)$$

A direct comparison between Eqs. (1) and (7) finally allows to recognize that

$$\sigma^{(s)} = - \left(\frac{q_i}{\theta^2} \right) \theta_{,i}. \quad (8)$$

¹ Whenever the internal energy is no longer the only one state-space variable (as it will be through this paper), Eq. (5) properly reads $\frac{\partial s}{\partial u} = \frac{1}{\theta}$.

In order to avoid any possible violation of the unilateral constraint (2), in the F-theory it is therefore sufficient to assume

$$q_i = -\lambda\theta_{,i} \quad (9)$$

as the constitutive equation for the heat flux (which is worldwide known as the F-law), if it is tacitly understood that the positive-valued constant λ means the thermal conductivity. The coupling of Eqs. (8) and (9), in fact, lets that the form of the specific-entropy production reads

$$\sigma^{(s)} = \left(\frac{\lambda}{\theta^2}\right)\theta_{,i}\theta_{,i} \quad (10)$$

from which it is easy matter to see that $\sigma^{(s)} = \sigma^{(s)}(u)$ is always a positive-definite function.

1.2 The Maxwell–Cattaneo theory

The Maxwell–Cattaneo (MC-) theory has been the first attempt to go beyond the validity's limits of the F-theory. Those limits are particularly evident when the heat transfer is a very fast and/or steep phenomenon (e.g., in the case of ultrasound propagation, the light scattering in gases, shock waves, etc.) [2,9,10], or whenever the relaxation time (i.e., the temporal lagging between the application of a temperature gradient and the appearance of a heat flux) becomes large enough to require a description of the transient regime [11].

According to the point of view of Extended Irreversible Thermodynamics (EIT) [2,7], in the MC-theory of heat transfer in a rigid body the state space is spanned by u and q_i ; from the physical point of view, this is tantamount to suppose that both the independent variations of u and q_i can, in principle, influence the consequent variations of the other thermodynamic fields, as for example the specific entropy.

Whereas u is still ruled by the balance law in Eq. (3), in this theory q_i can be no longer given by a constitutive relation (as it has been done in the case of the F-theory), but an evolution equation is needed for it. In order to theoretically derive it, we may observe that in the MC-theory $s = s(u, q_i)$ in such a way that in the framework of EIT the generalized Gibbs equation read [2,7]

$$ds = \left(\frac{1}{\theta}\right)du - \left(\frac{\tau_R q_i}{\lambda\theta^2}\right)dq_i \quad (11)$$

with the (positive) material function τ_R being the relaxation time of q_i , namely, the response time for the onset of the heat flow after a temperature gradient is suddenly imposed. That quantity is substantially the reciprocal of the frequency of resistive phonon collisions, i.e., the mechanisms of phonon scattering in which the phonons' energy is conserved, but not their momentum.² From Eq. (11) we have that the time derivative of s reads

$$\partial_t s = -\frac{q_{i,i}}{\theta} - \left(\frac{\tau_R q_i}{\lambda\theta^2}\right)\partial_t q_i \quad (12)$$

if Eq. (3) is employed. The use of the constitutive assumption in Eq. (6) allows then to rewrite Eq. (12) as

$$\partial_t s = -J_{i,i}^{(s)} - \frac{q_i}{\lambda\theta^2}(\lambda\theta_{,i} + \tau_R\partial_t q_i). \quad (13)$$

A direct comparison of Eqs. (1) and (13) yields

$$\sigma^{(s)} = -\frac{q_i}{\lambda\theta^2}(\lambda\theta_{,i} + \tau_R\partial_t q_i) \quad (14)$$

as the constitutive equation for the specific-entropy production. In order to guarantee the (thermodynamic) compatibility of the MC-theory with the unilateral constraint (2), it is still sufficient that $\sigma^{(s)} = \sigma^{(s)}(u, q_i)$ is a positive-definite function. For this reason in Eq. (14) we may set

$$q_i = -(\lambda\theta_{,i} + \tau_R\partial_t q_i) \quad (15)$$

² To be more precise we note that in EIT, when the generalized Gibbs equation is introduced, the function $\frac{\partial s}{\partial q_i}$ is firstly written in a very general form and then, by sequential comparisons, it is completely identified in terms of quantities which have their own clear physical meanings. For the rigorous derivation of Eq. (11) interested readers are therefore referred to Ref. [2] (see therein Part I—Subsec. 2.1.2). Therein comments about the degree of approximation of Eq. (11) can be also found.

which is also the required evolution equation of q_i and it is worldwide known as the MC-equation [12]. When Eq. (15) is introduced into Eq. (14), in fact, the following local form of the specific-entropy production for the heat transfer in a rigid body is recovered

$$\sigma^{(s)} = \frac{\lambda}{\theta^2} \left(\theta_{,i} + \frac{\tau_R}{\lambda} \partial_t q_i \right) \left(\theta_{,i} + \frac{\tau_R}{\lambda} \partial_t q_i \right) \quad (16)$$

in the case of the MC-theory. It seems worth noticing that Eqs. (15) and (16) reduce, respectively, to Eqs. (9) and (10) whenever $\tau_R \rightarrow 0$. From the above considerations, it arises that the MC-theory is compatible with the classical constitutive equation for $J_i^{(s)}$ [1], too.

1.3 Aims and scopes

The increasing interest in nanoscale heat-transport sciences led modern non-equilibrium thermodynamic theories to depart both from the F-theory, and from the MC-theory. Dealing with the heat transfer at nanoscale is not properly an easy task; from the theoretical point of view, to tackle with it several interesting approaches can be found in the literature, as it can be seen, for example, in the outstanding review by Guo and Wang [13]. All those approaches lie either on macroscopic, or mesoscopic, or microscopic methods. Among those methods, one spreading over a large span of time is the phonon hydrodynamics model, the usual starting point of which is the so-called Guyer–Krumhansl equation [2,14], i.e.,

$$\tau_R \partial_t q_i + q_i = -\lambda \theta_{,i} + \ell^2 (2q_{j,ji} + q_{i,jj}) \quad (17)$$

wherein ℓ is the mean-free path of phonons (i.e., quanta of the vibrational mechanical energy arising from oscillating atoms within a lattice) representing the heat carriers in dielectric solids. Equation (17) represents an interesting step beyond Eq. (15) (the latter recovered from the former whenever $\ell \rightarrow 0$, for example) since it is able to capture non-local effects in the heat transport, a topic of much interest at nanoscale wherein even small temperature differences may lead to high temperature gradients.

In nanosystems, indeed, also non-linear effects may strongly influence the electronic and optical properties: it could be, therefore, important to deeply examine them by introducing generalized nonlinear and non-local heat-transport equations [15]. Whereas the possibility of dealing with a non-local and non-linear model is clearly an important step toward a detailed and more refined description of the heat transfer at nanoscale, it has to be however noted that the introduction of non-linear terms may especially yield additional difficulties among which here we underline the correct setting-up of initial data (ID) and boundary conditions (BCs), which is of itself already a difficult task in the linear case (i.e., when only non-local effects are taken into account). In any model, in fact, both ID, and BCs should be always assigned in such a way that they have to be physically meaningful, besides correctly depicting the experimental reality, and the consequent initial-boundary value problem (IBVP) is mathematically consistent.

Along with the aforementioned observations, in the present paper:

- In Sect. 2, we derive a non-linear and non-local model of heat transfer in rigid nanosystems on macroscopic grounds and in agreement with the second law of thermodynamics. That model encompasses Eq. (17) as a special case. The aim of this section is to show how non-local and non-linear effects may naturally arise from Eq. (1).
- In Sect. 3, the above model, in its linear formulation, is employed to analytically solve an IBVP which sketches the propagation of second sound in one-dimensional (1D) nanosystems perturbed by a thermal shock. Therein a comparison with the analytical results arising from the MC-theory is also made. The aim of this section is twofold:
 1. to point out the possible influence of the relaxation times of higher-order fluxes, as well as the role played by non-local effects on second-sound propagation;
 2. to point out a plausible mathematical way of assigning ID and BCs which are both physically consistent, and depict the exact experimental situation under consideration.
- In Sect. 4 final comments and future perspectives are given.

2 Non-local and non-linear heat conduction in rigid solids

Whereas in a theoretical model (dealing with the heat-transfer phenomenon at nanoscale) the non-local effects may be introduced by the spatial derivatives of the state-space variables, the non-linear effects may be instead substantially understood in the following two different ways:

- (i) by letting the several material functions depend on the state-space variables [16, 17];
- (ii) by letting products between some state-space variables (or their spatial derivatives) directly enter the model equations [8, 18].

Here we especially aim at analyzing the consequence of the second type of nonlinear effects; thus, throughout this paper we assume constant values for all material functions.

Besides the specific internal energy u and the heat flux q_i , in our approach we also assume as independent (state-space) variable the flux of the heat flux Q_{ij} . Referring interested readers to Refs. [2, 7, 13, 19, 20] for exhaustive theoretical considerations about the physical interpretation of the second-order tensor Q_{ij} , here we only observe that within the kinetic theory of diluted gases one has

$$Q_{ij} = \int_{\mathbb{R}^3} \frac{m}{2} f(\mathbf{r}, \mathbf{C}, t) \|\mathbf{C}\|^2 C_i C_j d\mathbf{c}$$

wherein $f(\mathbf{r}, \mathbf{C}, t)$ is the distribution function (\mathbf{r} being the position of the generic particle and m its mass), and \mathbf{C} is the relative speed of the particles with respect to the barycentric velocity, with $\|\mathbf{C}\|$ being its modulus.³

Since Q_{ij} is a symmetric tensor we may split it into its deviatoric (traceless) part $\overset{\circ}{Q}_{ij}$ and its bulk part $Q\delta_{ij}$, namely, in the present theory we postulate that the state space is

$$\Sigma = \left\{ u, q_i, \overset{\circ}{Q}_{ij}, Q \right\}. \quad (18)$$

The basic idea underlying the above selection is that those fluxes, which are *genuinely* non-equilibrium quantities, constitute a rather natural way of accessing to a system through its boundary.

In agreement with both EIT [2, 7], and the Non-Equilibrium with Internal Variables [21], each of the above state-space variables has to be characterized by its own evolution equation. Recalling that the time rate of u is given by Eq. (3), in this section we therefore derive the evolution equations for the above (state-space) flux variables. To do this, we start to observe that the very general form of the constitutive equation of the specific entropy is

$$s = s\left(u, q_i, \overset{\circ}{Q}_{ij}, Q\right)$$

owing to Eq. (18). For this reason, in agreement with EIT (see Part III—Subsec. 9.3.2 in Ref. [2]), in our approach we generalize the Gibbs equation (11) as

$$ds = \left(\frac{1}{\theta}\right) du - \left(\frac{\tau_R q_i}{\lambda\theta^2}\right) dq_i - \left[\left(\frac{\tau_R \overset{\circ}{Q}_{ij}}{2\lambda\theta^2}\right) \frac{\partial}{\partial\theta} \left(\frac{\theta\tau_1}{\eta_1}\right)\right] d\overset{\circ}{Q}_{ij} - \left[\left(\frac{\tau_R Q}{\lambda\theta^2}\right) \frac{\partial}{\partial\theta} \left(\frac{\theta\tau_0}{\eta_0}\right)\right] dQ \quad (19)$$

wherein the two (positive-valued) material functions τ_1 and τ_0 mean the relaxation times of $\overset{\circ}{Q}_{ij}$ and Q , respectively, and account for the relaxation effects of the higher-order fluxes [2, 7]. In some situations, as for example in diluted gases, the relaxation times of higher-order fluxes are of the same order as that of the heat flux itself, in such a way that when q_i is taken as an independent variable, all higher-order fluxes should also be taken into account. Further considerations about τ_1 and τ_0 are postponed to Sect. 2.2.

At the present stage, we leave undetermined the other two quantities η_0 and η_1 entering Eq. (19). They however will be clearly identified in Sect. 2.1. For our scope it is enough to claim that they are positive quantities.

³ It seems worth noticing that in the present paper we assume that Q_{ij} has the unit of $\text{Wm}^{-1} \text{s}^{-1}$ along with Ref. [19] (see therein Sec. 2) and Ref. [2] (see therein Part III—Subsec. 9.3.1), for example. In Ref. [7], instead, Q_{ij} has the unit of Wm^{-1} (see therein Subsec. 7.1.3).

The properties of $\overset{\circ}{Q}_{ij}$ and Q allow to suppose that the ratios $\frac{\tau_1}{\eta_1}$ and $\frac{\tau_0}{\eta_0}$ remain constant [2], as it will be shown in Sect. 2.2. As a consequence of this from Eq. (19) we may formally obtain the following time derivative of s :

$$\partial_t s = -\frac{q_{i,i}}{\theta} - q_i \left(\frac{\tau_R}{\lambda\theta^2}\right) \partial_t q_i - \overset{\circ}{Q}_{ij} \left(\frac{\tau_R\tau_1}{2\eta_1\lambda\theta^2}\right) \partial_t \overset{\circ}{Q}_{ij} - Q \left(\frac{\tau_R\tau_0}{\eta_0\lambda\theta^2}\right) \partial_t Q. \tag{20}$$

If we go beyond the classical constitutive assumption in Eq. (6) and therefore further suppose

$$J_i^{(s)} = \frac{q_j}{\theta} \left[\left(1 - \frac{\tau_R Q}{\lambda\theta}\right) \delta_{ij} - \frac{\tau_R \overset{\circ}{Q}_{ij}}{\lambda\theta} \right] \tag{21}$$

according to EIT [2], by direct calculations Eq. (20) can be also rewritten as

$$\begin{aligned} \partial_t s = & -J_{i,i}^{(s)} - \frac{q_i}{\lambda\theta^2} \left\{ \lambda \left[\left(1 - \frac{2\tau_R Q}{\lambda\theta}\right) \delta_{ij} - \frac{2\tau_R \overset{\circ}{Q}_{ij}}{\lambda\theta} \right] \theta_{,j} + \tau_R \left(\partial_t q_i + Q_{,i} + \overset{\circ}{Q}_{ij,j} \right) \right\} \\ & - \overset{\circ}{Q}_{ij} \left(\frac{\tau_R}{2\eta_1\lambda\theta^2}\right) \left[\tau_1 \partial_t \overset{\circ}{Q}_{ij} + 2\eta_1 \left(q_{i,j}^{\text{sym}} \right) \right] - Q \left(\frac{\tau_R}{\eta_0\lambda\theta^2}\right) (\tau_0 \partial_t Q + \eta_0 q_{i,j} \delta_{ij}). \end{aligned} \tag{22}$$

By comparing Eqs. (1) and (22) we may then point out the following constitutive equation for the specific-entropy production:

$$\begin{aligned} \sigma^{(s)} = & -\frac{q_i}{\lambda\theta^2} \left\{ \lambda \left[\left(1 - \frac{2\tau_R Q}{\lambda\theta}\right) \delta_{ij} - \frac{2\tau_R \overset{\circ}{Q}_{ij}}{\lambda\theta} \right] \theta_{,j} + \tau_R \left(\partial_t q_i + Q_{,i} + \overset{\circ}{Q}_{ij,j} \right) \right\} \\ & - \overset{\circ}{Q}_{ij} \left(\frac{\tau_R}{2\eta_1\lambda\theta^2}\right) \left[\tau_1 \partial_t \overset{\circ}{Q}_{ij} + 2\eta_1 \left(q_{i,j}^{\text{sym}} \right) \right] - Q \left(\frac{\tau_R}{\eta_0\lambda\theta^2}\right) (\tau_0 \partial_t Q + \eta_0 q_{i,j} \delta_{ij}). \end{aligned} \tag{23}$$

Note that Eq. (23) encompasses Eq. (14) as a special case: in fact, the latter form of $\sigma^{(s)}$ is obtained by the former form of $\sigma^{(s)}$ whenever $\overset{\circ}{Q}_{ij} \rightarrow 0$ and $Q \rightarrow 0$.

In order to guarantee that the unilateral constraint (2) is always fulfilled, it is sufficient to make assumptions letting the function $\sigma^{(s)}$ be positive definite. Since Eq. (23) substantially displays the bilinear form

$$\sigma^{(s)} = A q_i X_i + B \overset{\circ}{Q}_{ij} X_{ij} + C Q X \tag{24}$$

wherein A , B and C are strictly negative coefficients, whereas the following quantities

$$X_i = \lambda \left[\left(1 - \frac{2\tau_R Q}{\lambda\theta}\right) \delta_{ij} - \frac{2\tau_R \overset{\circ}{Q}_{ij}}{\lambda\theta} \right] \theta_{,j} + \tau_R \left(\partial_t q_i + Q_{,i} + \overset{\circ}{Q}_{ij,j} \right) \tag{25a}$$

$$X_{ij} = \tau_1 \partial_t \overset{\circ}{Q}_{ij} + 2\eta_1 \left(q_{i,j}^{\text{sym}} \right) \tag{25b}$$

$$X = \tau_0 \partial_t Q + \eta_0 q_{i,j} \delta_{ij} \tag{25c}$$

are the so-called thermodynamic forces [1,2], a possible way of fulfilling Eq. (2) in any situation is to assume

$$X_i = -q_i \tag{26a}$$

$$X_{ij} = -\overset{\circ}{Q}_{ij} \tag{26b}$$

$$X = -Q \tag{26c}$$

for example. The assumptions in Eqs. (26) straightforwardly lead to

$$\partial_t q_i = -\frac{q_i}{\tau_R} - \frac{\lambda}{\tau_R} \left[\left(1 - \frac{2\tau_R Q}{\lambda\theta} \right) \delta_{ij} - \frac{2\tau_R \overset{\circ}{Q}_{ij}}{\lambda\theta} \right] \theta_{,j} - \overset{\circ}{Q}_{ij,j} - Q_{,i} \quad (27a)$$

$$\partial_t \overset{\circ}{Q}_{ij} = -\frac{\overset{\circ}{Q}_{ij}}{\tau_1} - \left(\frac{2\eta_1}{\tau_1} \right) \left(q_{i,j}^{\text{sym}} \right) \quad (27b)$$

$$\partial_t Q = -\frac{Q}{\tau_0} - \left(\frac{\eta_0}{\tau_0} \right) q_{i,j} \delta_{ij}. \quad (27c)$$

2.1 The model equations

Provided the physical meanings of η_0 and η_1 are given, Eqs. (27) are proper the evolution equations of the (state-space) flux variables we're searching for. In order to make those identifications, indeed, we may start to observe that whenever both $\partial_t \overset{\circ}{Q}_{ij} \rightarrow 0$, and $\partial_t Q \rightarrow 0$, the insertion of Eqs. (27b) and (27c) into Eq. (27a) turns out

$$\tau_R \partial_t q_i + q_i = -\Lambda_{ij}^{\text{eff}} \theta_{,j} + 2\eta_1 \left(q_{i,j}^{\text{sym}} \right)_{,j} + \eta_0 q_{j,ji} \quad (28)$$

wherein the second-order tensor

$$\Lambda_{ij}^{\text{eff}} = \lambda \left[\left(1 - \frac{2\tau_R Q}{\lambda\theta} \right) \delta_{ij} - \frac{2\tau_R \overset{\circ}{Q}_{ij}}{\lambda\theta} \right] \quad (29)$$

can be substantially meant as an effective thermal conductivity (which could be related to the compelling problem of flux limiters [22–24]). Whenever the non-equilibrium-temperature approximation [2, 16] holds, namely, if one has

$$ds = \left(\frac{1}{\theta} \right) du - \left(\frac{\tau_R q_i}{\lambda\theta_{\text{eq}}^2} \right) dq_i - \left[\left(\frac{\tau_R \overset{\circ}{Q}_{ij}}{2\lambda\theta_{\text{eq}}^2} \right) \frac{\partial}{\partial \theta} \left(\frac{\theta\tau_1}{\eta_1} \right) \right] d\overset{\circ}{Q}_{ij} - \left[\left(\frac{\tau_R Q}{\lambda\theta_{\text{eq}}^2} \right) \frac{\partial}{\partial \theta} \left(\frac{\theta\tau_0}{\eta_0} \right) \right] dQ$$

and

$$J_i^{(s)} = \frac{q_j}{\theta} \left[\left(1 - \frac{\tau_R Q}{\lambda\theta_{\text{eq}}} \right) \delta_{ij} - \frac{\tau_R \overset{\circ}{Q}_{ij}}{\lambda\theta_{\text{eq}}} \right]$$

with θ_{eq} being the (constant value of the) local-equilibrium temperature, instead of Eqs. (19) and (21), respectively, the non-linear terms proportional to $\overset{\circ}{Q}_{ij} \theta_{,j}$ and $Q\theta_{,i}$ vanish and the effective thermal conductivity above reduces to the bulk thermal conductivity. In that case, moreover, it is easy matter to observe that Eqs. (17) and (28) coincide provided the following identifications hold:

$$\eta_1 = \frac{\ell^2}{\tau_R} \quad (30a)$$

$$\eta_0 = \frac{5\ell^2}{3\tau_R}. \quad (30b)$$

Equations (30) turn out the expressions of η_1 and η_0 in terms of clear physical quantities. If the assumptions in Eqs. (30) are made, from the local balance of energy (3) and Eqs. (27) we finally have

$$\partial_t u = -q_{i,i} \quad (31a)$$

$$\partial_t q_i = -\frac{q_i}{\tau_R} - \frac{\lambda}{\tau_R} \left[\left(1 - \frac{2\tau_R Q}{\lambda\theta} \right) \delta_{ij} - \frac{2\tau_R \overset{\circ}{Q}_{ij}}{\lambda\theta} \right] \theta_{,j} - \overset{\circ}{Q}_{ij,j} - Q_{,i} \quad (31b)$$

$$\partial_t \overset{\circ}{Q}_{ij} = -\frac{\overset{\circ}{Q}_{ij}}{\tau_1} - \left(\frac{2\ell^2}{\tau_R \tau_1} \right) \left(q_{i,j}^{\text{sym}} \right) \quad (31c)$$

$$\partial_t Q = -\frac{Q}{\tau_0} - \left(\frac{5\ell^2 \delta_{ij}}{3\tau_0 \tau_R} \right) q_{i,j} \quad (31d)$$

which are our model equations.

2.2 Comparison with the 9-moment theory

When the non-equilibrium-temperature approximation holds Eqs. (31) become

$$\partial_t u = -q_{i,i} \quad (32a)$$

$$\partial_t q_i = -\frac{q_i}{\tau_R} - \frac{\lambda}{\tau_R c_v} u_{,i} - \overset{\circ}{Q}_{ij,j} - Q_{,i} \quad (32b)$$

$$\partial_t \overset{\circ}{Q}_{ij} = -\frac{\overset{\circ}{Q}_{ij}}{\tau_1} - \left(\frac{2\ell^2}{\tau_R \tau_1} \right) \left(q_{i,j}^{\text{sym}} \right) \quad (32c)$$

$$\partial_t Q = -\frac{Q}{\tau_0} - \left(\frac{5\ell^2 \delta_{ij}}{3\tau_0 \tau_R} \right) q_{i,j} \quad (32d)$$

once the classical thermodynamic relation

$$c_v = \frac{\partial u}{\partial \theta} \quad (33)$$

is used, with c_v being the specific heat at constant volume per unit volume (always larger than zero, as experimental evidences point out).

We may indeed recognize that the model in Eqs. (32) is closely related to the model which characterizes the 9-moment theory [25], i.e., to the model based upon

$$\partial_t u = -\|\mathbf{c}\|^2 p_{i,i} \quad (34a)$$

$$\partial_t p_i = -\frac{p_i}{\tau_R} - \frac{1}{3} u_{,i} - \overset{\circ}{N}_{ij,j} \quad (34b)$$

$$\partial_t \overset{\circ}{N}_{ij} = -\frac{\overset{\circ}{N}_{ij}}{\tau_\star} - \frac{2}{5} \|\mathbf{c}\|^2 \left(p_{i,j}^{\text{sym}} \right) \quad (34c)$$

wherein $\|\mathbf{c}\|$ means the modulus of the phonons' Debye speed (defined as some mean value of longitudinal and transversal speed of sound), and

$$p_i = \hbar \int_{\mathbb{R}^3} k_i f(\mathbf{x}, t, \mathbf{k}) d\mathbf{k} \quad (35a)$$

$$\overset{\circ}{N}_{ij} = \hbar \|\mathbf{c}\| \int_{\mathbb{R}^3} \frac{1}{\|\mathbf{k}\|} k_i k_j f(\mathbf{x}, t, \mathbf{k}) d\mathbf{k} - \frac{u}{3} \delta_{ij} \quad (35b)$$

with \hbar being the Planck's constant, \mathbf{k} being the wave vector (the modulus of which is $\|\mathbf{k}\|$), the function $f(\mathbf{x}, t, \mathbf{k})$ means the phase density. The relaxation time τ_\star appearing in Eqs. (34) is such that

$$\frac{1}{\tau_\star} = \frac{1}{\tau_R} + \frac{1}{\tau_N} \quad (36)$$

where τ_N means the reciprocal of the frequency of normal phonon collisions, i.e., the mechanisms of phonon scattering in which both the phonons' energy, and their momentum is conserved. By comparing Eqs. (32) and (34), indeed, it is possible to set the following parallelisms

$$q_i \longleftrightarrow p_i \quad (37a)$$

$$Q_{ij} \longleftrightarrow N_{ij} \quad (37b)$$

between the field variables involved in those models, the only difference being the form of the isotropic part of the two symmetric second-order tensors Q_{ij} and N_{ij} , which in the latter case is only related to u , as it follows from Eq. (35b). The parallelism between Eqs. (32) and (34), besides giving a common root (very well defined in the kinetic theory) to our model and the 9-moment theory, allows us to give a deeper physical insight into the relaxation times τ_1 and τ_0 : both of them, in fact, should be related to the relaxation time τ_* defined by Eq. (36) which is tantamount to claim that the relaxation times of higher-order fluxes in our model are related both to the resistive scatterings, and to the normal scatterings.

The above considerations justify the assumption of constant values for the ratios $\frac{\tau_1}{\eta_1}$ and $\frac{\tau_0}{\eta_0}$ that we have made in Sect. 2. If Eqs. (30) hold, in fact, the above parallelism allows us to state that both $\frac{\tau_1}{\eta_1}$, and $\frac{\tau_0}{\eta_0}$ are proportional to $\|\mathbf{c}\|^2$, which can be surely supposed to be constant.

3 Second-sound propagation

In the present section we investigate the second-sound propagation predicted by the theoretical model in Eqs. (31). To this end, for computational needs, we introduce the following dimensionless variables:

$$\begin{aligned} \mathbf{x}_i &= \frac{x_i}{L} & \mathbf{t} &= \frac{t}{\tau_R} \\ \mathbb{T} &= \frac{\theta - T_0}{T_0} & \mathbf{h}_i &= \frac{L}{\lambda T_0} q_i & \mathring{\mathbf{H}}_{ij} &= \frac{\tau_1}{\lambda T_0} \mathring{Q}_{ij} & \mathbf{H} &= \frac{\tau_0}{\lambda T_0} Q \end{aligned} \quad (38)$$

with L being the characteristic length of our system, and T_0 a suitable reference temperature (e.g., the initial temperature of the system). For our goal, we also make use of Eq. (33) such that Eqs. (32a) can be rewritten in terms of the time variation of non-equilibrium temperature θ . In this way Eq. (31) become

$$\partial_t \mathbb{T} + \frac{\text{Kn}^2}{3} \mathbf{h}_{k,k} = 0 \quad (39a)$$

$$\partial_t \mathbf{h}_i + \mathbf{h}_i + \left\{ \left[1 - \frac{2\mathbf{H}}{\alpha(1+\mathbb{T})} \right] \delta_{ij} - \frac{2\mathring{\mathbf{H}}_{ij}}{\beta(1+\mathbb{T})} \right\} \mathbb{T}_{,j} + \frac{\mathring{\mathbf{H}}_{ij,j}}{\beta} + \frac{\mathbf{H}_{,i}}{\alpha} = 0 \quad (39b)$$

$$\partial_t \mathring{\mathbf{H}}_{ij} + \frac{\mathring{\mathbf{H}}_{ij}}{\beta} + \text{Kn}^2 \left(\mathbf{h}_{i,j} + \mathbf{h}_{j,i} - \frac{2\delta_{ij}}{3} \mathbf{h}_{k,k} \right) = 0 \quad (39c)$$

$$\partial_t \mathbf{H} + \frac{\mathbf{H}}{\alpha} + \frac{5\text{Kn}^2}{3} \mathbf{h}_{k,k} = 0 \quad (39d)$$

wherein we set $\tau_0 = \alpha\tau_R$, $\tau_1 = \beta\tau_R$, and $\text{Kn} = \frac{\ell}{L}$ stands for the Knudsen number.⁴ According to what previously said, therefore, in the present analysis the non-dimensional coefficients α and β account for the relaxation effects of the higher-order fluxes (related both to the resistive scatterings, and to the normal ones), whereas Kn introduces non-local effects.

In closing this part, we note that in deriving Eqs. (39) we estimated the resistive relaxation time of phonons as

$$\tau_R = \frac{\ell}{V_0} \quad (40)$$

⁴ We note that in the case of nanoscale heat transfer one usually has $\text{Kn} \sim \mathcal{O}(1)$ (i.e., $\ell \geq L$), whereas the case $\text{Kn} \rightarrow 0^+$ (i.e., $\ell \ll L$) corresponds to the case of macroscale heat transfer.

with V_0 standing for the average phonon speed (measured at the reference temperature-value T_0), and we used the well-known *Ziman limit* [26] for the thermal conductivity, i.e.,

$$\lambda = \frac{c_v \tau_R V_0^2}{3} \quad (41)$$

as it is usually assumed in the hydrodynamic theory of second-sound propagation in insulators. Although the assumptions in Eqs. (40) and (41) may lead to a quantitative inaccuracy, it is clear that the results obtained below are not critically dependent upon those assumptions.

3.1 The mathematical formulation

Here we put ourselves in the 1D case for the sake of simplicity. From the physical point of view this means that we are only interested in the thermal transport within 1D (indefinitely long) nanostructures (e.g., nanowires, nanofibers, nanotubes, and nanorods) which represent one of the best-defined and controlled classes of nanoscale building blocks. We refer to Refs. [27,28] and the references cited therein for some comprehensive reviews about the use of these material systems.

Dealing with Eqs. (39) is not properly an easy task, at least if one is searching for analytical solutions which can depict the experimental evidences. One of the main problems in dealing with Eqs. (39) lies, for example, on the question regarding ID and BCs and the way they have to be correctly assigned, as it has been previously observed in Sect. 1. For this reason, as a first attempt to a more general analysis, to reduce our computations to a simpler level, here we put ourselves in the non-equilibrium-temperature approximation and therefore we neglect the terms proportional to $\overset{\circ}{H}_{ij} \bar{T}_{,j}$ and $\overset{\circ}{H} T_{,j}$ in Eq. (39b). By indicating with x the sole (non-dimensional) Cartesian coordinate, as a consequence of the assumptions above, Eqs. (39) reduce to

$$\partial_t T + \frac{\text{Kn}^2}{3} \partial_x h_x = 0 \quad (42a)$$

$$\partial_t h_x + h_x + \partial_x T + \frac{\partial_x \overset{\circ}{H}_{xx}}{\beta} + \frac{\partial_x H}{\alpha} = 0 \quad (42b)$$

$$\partial_t \overset{\circ}{H}_{xx} + \frac{\overset{\circ}{H}_{xx}}{\beta} + \frac{4 \text{Kn}^2}{3} \partial_x h_x = 0 \quad (42c)$$

$$\partial_t H + \frac{H}{\alpha} + \frac{5 \text{Kn}^2}{3} \partial_x h_x = 0. \quad (42d)$$

The above system of coupled PDEs will be solved by prescribing the following ID

$$\begin{aligned} T(x, 0) &= 0 & \forall x \in [0, +\infty) \\ h_x(x, 0) &= 0 & \forall x \in [0, +\infty) \\ \overset{\circ}{H}_{xx}(x, 0) &= 0 & \forall x \in [0, +\infty) \\ H(x, 0) &= 0 & \forall x \in [0, +\infty) \end{aligned} \quad (43)$$

which, from the physical point of view, mean that our rigid conductor is initially at equilibrium and at the reference temperature T_0 . Moreover, we also assign the following BCs

$$T(0, t) = T \bullet \mathcal{H}(t) \quad T(+\infty, t) = 0 \quad \forall t \in (0, +\infty) \quad (44)$$

wherein \mathcal{H} is the Heaviside unit step function. This is tantamount to mathematically depicting the practical situation in which at the time $t = 0^+$ the domain boundary at $x = 0$ is only affected by a step-jump in temperature. The neglect of non-linear terms has allowed us to not assign any BCs for the other unknown functions $h_x(x, t)$, $\overset{\circ}{H}_{xx}(x, t)$ and $H(x, t)$: we let, in this way, the model furnish the values of those functions also at the boundary. Otherwise, we would have had to assign those BCs, thus incurring the problem of the

physical meaning of the prescribed values for the unknown functions at the boundary, a problem which is still open.⁵

The IBVP in Eqs. (42)–(44), therefore, is able to describe the behavior of an infinite 1D nanosystem which is perturbed from its initial equilibrium state by a thermal pulse (i.e., a thermal shock) applied in its left-hand side end. From the practical point of view, in Eq. (44) $\mathbf{T}^\bullet \in \mathbb{R}^+$ stands for a dimensionless constant which captures the energy amount of the thermal shock perturbing the system at hand. Further comments about the ID in Eqs. (43) and the BCs in Eq. (44) will be made in Sect. 3.3.

3.2 The form of the basic fields

The approximate analytical solution of the IBVP in Eqs. (42)–(44) is the following:

$$T(x, t) = \left[\mathbf{T}^\bullet e^{-\frac{\zeta \epsilon}{\text{Kn}} x} \right] \mathcal{H} \left(t - \frac{\zeta}{\text{Kn}} x \right) \quad (45a)$$

$$h(x, t) = \frac{3\mathbf{T}^\bullet e^{-\frac{\zeta \epsilon}{\text{Kn}} x}}{\zeta \text{Kn}} \left[1 - \epsilon \left(t - \frac{\zeta}{\text{Kn}} x \right) \right] \mathcal{H} \left(t - \frac{\zeta}{\text{Kn}} x \right) \quad (45b)$$

$$\overset{\circ}{H}_{xx}(x, t) = 4\mathbf{T}^\bullet e^{-\frac{\zeta \epsilon}{\text{Kn}} x} \left[e^{-\frac{1}{\beta} \left(t - \frac{\zeta}{\text{Kn}} x \right)} \right] \mathcal{H} \left(t - \frac{\zeta}{\text{Kn}} x \right) \quad (45c)$$

$$H(x, t) = 5\mathbf{T}^\bullet e^{-\frac{\zeta \epsilon}{\text{Kn}} x} \left[e^{-\frac{1}{\alpha} \left(t - \frac{\zeta}{\text{Kn}} x \right)} \right] \mathcal{H} \left(t - \frac{\zeta}{\text{Kn}} x \right) \quad (45d)$$

wherein we have set

$$\zeta = \sqrt{\frac{3\alpha\beta}{\alpha\beta + 4\alpha + 5\beta}} \quad (46a)$$

$$\epsilon = \frac{1}{2} \left(1 + \frac{1}{\alpha\beta} \cdot \frac{4\alpha^2 + 5\beta^2}{\alpha\beta + 4\alpha + 5\beta} \right) \quad (46b)$$

just for the sake of a compact notation. Interested readers can refer to “Appendix” at the end of this paper for a sketch of the solution method used to obtain the form of the basic fields in Eqs. (45); therein considerations about the degree of approximation of Eqs. (45) are also made. Here, instead, we aim at drawing the attention on some consequences arising from Eqs. (45).

In Fig. 1, we plot the theoretical behavior of the non-dimensional temperature T arising from Eq. (45a) when $\alpha = \beta = 1$, $\mathbf{T}^\bullet = 1$ and $\text{Kn} = 1$ (just for the sake of computational needs). That figure clearly displays the propagating temperature wave (so pointing out the hyperbolic behavior of Sys. (39) in the 1D linear case): in fact, only the region before the front wave is perturbed (i.e., therein $T \neq 0$) whereas the region ahead the front wave is still in equilibrium (i.e., therein $T = 0$). Owing to dissipative effects, from Fig. 1 it is also possible to see how the energy amount of the thermal wave progressively shrinks for increasing time.

In the case of Eq. (45a), it seems also interesting to observe that the dissipative effects are influenced both by the relaxation times of Q and $\overset{\circ}{Q}_{ij}$ (accounted by α and β , respectively), and by the phonon mean-free path (accounted by Kn).

In particular, we may infer that the temperature-wave energy amount

- decreases as steeper as α and β reduce. This can be seen, for example, in Fig. 2 wherein the temperature T behavior, as a function of the distance x from the thermal-shock source, is investigated for different values of α and β .
- decreases as steeper as Kn reduces. This can be seen, for example, in Fig. 3 wherein the temperature T behavior, as a function of the distance x from the thermal-shock source, is investigated for different values of Kn .

⁵ In Ref. [2] interesting considerations can be found in this regard (see therein Box 9.1 in page 213).

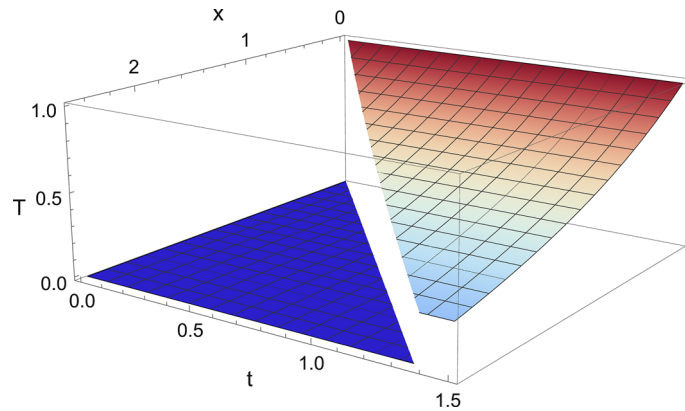


Fig. 1 T versus x and t : analytical solution arising from Eq. (45a). Data caption: $\alpha = \beta = 1$; $T^\bullet = 1$; $Kn = 1$. The jump discontinuity therein represents the propagating front of the temperature wave.

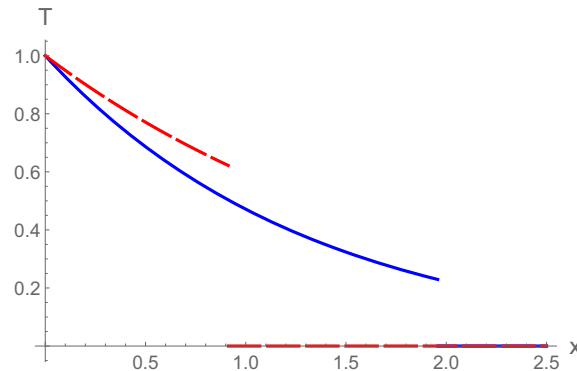


Fig. 2 T versus x as a function of α and β : theoretical behavior arising from Eq. (45a). In more detail, in figure the dashed (red) curve arises when $\alpha = \beta = 1$, and the solid (blue) curve arises when $\alpha = \beta = 0.2$. Data caption: $t = 0.5$; $T^\bullet = 1$; $Kn = 1$. The jump discontinuity therein occurs at the front of the moving temperature wave.

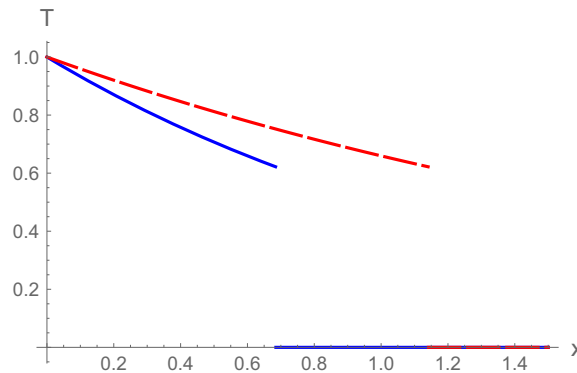


Fig. 3 T versus x as a function of Kn : theoretical behavior arising from Eq. (45a). In more detail, in figure the dashed (red) curve arises when $Kn = 1.25$, and the solid (blue) curve arises $Kn = 0.75$. Data caption: $t = 0.5$; $\alpha = \beta = 1$; $T^\bullet = 1$. The jump discontinuity therein occurs at the front of the moving temperature wave.

3.3 Results arising from the entropy balance

From the mathematical point of view, it is clear that the form of the basic fields in Eqs. (45) strictly depends on the model in Eqs. (42), as well as on the ID in Eqs. (43) and on the BCs in Eq. (44). Here we avoid deepening too much into the mathematical details (Eqs. (45) are however an implicit proof of the existence of the solution of the IBVP in Eqs. (42)–(44)), and only look at the physical meaning of Eqs. (43) and (44).

From the practical point of view, we stress that both ID, and BCs should arise from experimental evidences and have their own physical clear meaning. The determination of the initial conditions is generally of no concern either in steady-state situations, or in transient problems, since it is usually admitted that the system at hand is initially in a thermodynamic equilibrium. This is the main reason why ID have been given by Eqs. (43). The right setting-up of BCs, instead, is in general more delicate and controversial. It has to be also noted that in the case of Eqs. (42) the above problem becomes still more acute since therein the four unknown fields $T(x, t)$, $h_x(x, t)$, $\overset{\circ}{H}_{xx}(x, t)$ and $H(x, t)$ are coupled.

As a consequence, the following questions may naturally arise: is the IBVP in Eqs. (42)–(44) physically consistent? Since in Sect. 3.1 only the value of the unknown function $T(x, t)$ at the boundary has been given, are the BCs in Eq. (44) admissible? Whereas the results contained in Sect. 2 make us sure about the physical validity of the theoretical model in Eqs. (42), to answer the above questions in the present section we analyze the consequences of the unilateral constraint (2). In particular, if we introduce the following further dimensionless quantities

$$G_i^{(s)} = \frac{L}{\lambda} J_i^{(s)} \quad \Sigma^{(s)} = \frac{L^2}{\lambda} \sigma^{(s)} \tag{47}$$

from Eqs. (21) and (23), respectively, we have

$$G_i^{(s)} = \frac{h_j}{1+T} \left\{ \left[1 - \frac{H}{\alpha(1+T)} \right] \delta_{ij} - \frac{\overset{\circ}{H}_{ij}}{\beta(1+T)} \right\} \tag{48a}$$

$$\begin{aligned} \Sigma^{(s)} = & -\frac{1}{(1+T)^2} \left\{ h_i \left[T_{,i} - \frac{2HT_{,i}}{\alpha(1+T)} - \frac{2\overset{\circ}{H}_{ij}T_{,j}}{\beta(1+T)} + \partial_t h_i + \frac{\overset{\circ}{H}_{ij,j}}{\beta} + \frac{H_{,i}}{\alpha} \right] \right. \\ & \left. + \overset{\circ}{H}_{ij} \left[\frac{\partial_t \overset{\circ}{H}_{ij}}{2\beta Kn^2} + \frac{1}{2\beta} (h_{i,j} + h_{j,i} - \frac{2\delta_{ij}}{3} h_{k,k}) \right] + H \left(\frac{3\partial_t H}{5\alpha Kn^2} + \frac{h_{k,k}}{\alpha} \right) \right\}. \end{aligned} \tag{48b}$$

By neglecting the non-linear terms proportional to $HT_{,j}$ and $\overset{\circ}{H}_{ij}T_{,j}$ in Eq. (48b), in the 1D case we have

$$G_x^{(s)} = \frac{h_x}{1+T} \left[1 - \frac{H}{\alpha(1+T)} - \frac{\overset{\circ}{H}_{xx}}{\beta(1+T)} \right] \tag{49a}$$

$$\begin{aligned} \Sigma^{(s)} = & -\frac{1}{(1+T)^2} \left[h_x \left(\partial_x T + \partial_t h_x + \frac{\partial_x \overset{\circ}{H}_{xx}}{\beta} + \frac{\partial_x H}{\alpha} \right) \right. \\ & \left. + \overset{\circ}{H}_{xx} \left(\frac{\partial_t \overset{\circ}{H}_{xx}}{2\beta Kn^2} + \frac{2\partial_x h_x}{3\beta} \right) + H \left(\frac{3\partial_t H}{5\alpha Kn^2} + \frac{\partial_x h_x}{\alpha} \right) \right]. \end{aligned} \tag{49b}$$

In Fig. 4, we plot the theoretical behavior of the non-dimensional specific-entropy production $\Sigma^{(s)}$ arising from Eq. (49b) when $\alpha = \beta = 1$, $T^\bullet = 1$ and $Kn = 1$ (just for the sake of computational needs). As it was expected, Fig. 4 shows that only the (out-of-equilibrium) region before the front wave is characterized by $\Sigma^{(s)}$ values different from zero (but strictly positive, according to second law of thermodynamics). In the region ahead the front wave, which is instead still at equilibrium, it obviously holds $\Sigma^{(s)} = 0$. The behavior of $\Sigma^{(s)}$ is monotonically decreasing: this is logical since in time the temperature wave progressively loses its energy amount, as observed in Sect. 3.2.

The above considerations are enough to claim the validity of the physical setting of the phenomenon at hand, i.e., Eqs. (43) and (44).

3.4 Comparison with the MC-theory

The limits of F-theory, which are well known since decades, have led to several interesting generalizations of it. Those generalizations are obviously not unique: they generally differ in the underlying physical principles

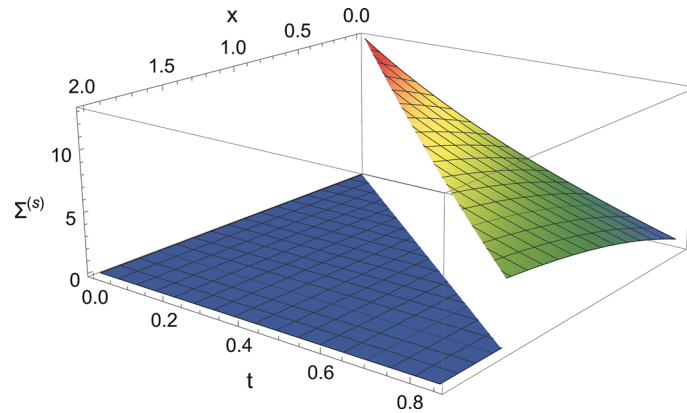


Fig. 4 $\Sigma^{(s)}$ versus x and t : analytical solution arising from Eq. (49b). Data caption: $\alpha = \beta = 1$; $T^\bullet = 1$; $Kn = 1$. The jump discontinuity therein occurs at the front of the moving temperature wave

and in modeling capabilities. In Ref. [21], for example, two theoretical models are discussed and compared: one based upon Rational Extended Thermodynamics, and the other one based upon Non-Equilibrium Thermodynamics with Internal Variables. In Ref. [29], instead, the Grad-13 equations [30] have been embedded into the framework of GENERIC [31]. Since the comparison between different theories is surely one of the major stimuli both to enhance previous models, and to find new others, by means of the second-sound propagation in this part we compare the results of Sect. 3 with those arising from the MC-theory. The MC-theory is considered here only for the fact that it can be recovered (as special case) from any theory beyond the F-law. We postpone to future works a more complete and refined comparison between the different models proposed in the literature.

Since in the MC-theory the two basic fields $\overset{\circ}{H}_{xx}(x, t)$ and $H(x, t)$ are not taken into account (according to what previously said in Sect. 1.2), then in that theory the IBVP given by Eqs. (42)–(44) reduces to

$$\partial_t T + \frac{Kn^2}{3} \partial_x h_x = 0 \tag{50a}$$

$$\partial_t h_x + h_x + \partial_x T = 0 \tag{50b}$$

$$T(x, 0) = 0 \quad \forall x \in [0, +\infty) \tag{50c}$$

$$h_x(x, 0) = 0 \quad \forall x \in [0, +\infty) \tag{50d}$$

$$T(0, t) = T^\bullet \mathcal{H}(t) \quad T(+\infty, t) = 0 \quad \forall t \in (0, +\infty) \tag{50d}$$

in such a way that one would have the following analytical solutions

$$T(x, t) = \left[T^\bullet e^{-\frac{\sqrt{3}}{2Kn}x} \right] \mathcal{H} \left(t - \frac{\sqrt{3}}{Kn}x \right) \tag{51a}$$

$$h(x, t) = \frac{\sqrt{3}T^\bullet e^{-\frac{\sqrt{3}}{2Kn}x}}{Kn} \left[1 - \frac{1}{2} \left(t - \frac{\sqrt{3}}{Kn}x \right) \right] \mathcal{H} \left(t - \frac{\sqrt{3}}{Kn}x \right) \tag{51b}$$

instead of Eqs. (45a) and (45b). A sketch of the solution method used to obtain the form of the basic fields in Eqs. (51) can be found in “Appendix,” too.

In Fig. 5, we compare the behaviors of the analytical solutions in Eqs. (45a) and (51a) when $t = 0.5$, $\alpha = \beta = 1$, $T^\bullet = 1$, and $Kn = 1$ just for the sake of computation. It clearly points out that the temperature wave predicted by Eq. (45a) (i.e., the dashed red curve therein) is faster than the temperature wave predicted by Eq. (51a) (i.e., the solid blue curve therein): in the former case, in fact, the front wave (characterized by the jump discontinuity) is placed at a distance larger than that at which the front wave in the latter case occurs. This result was indeed expected since the second-sound speed predicted by Eqs. (31) is larger than that predicted by the MC-theory [2,32], whatever the values of the parameter α , β and Kn are.

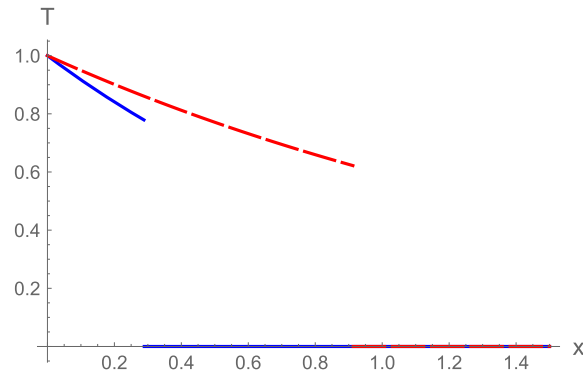


Fig. 5 T versus x : analytical solutions arising from Eqs. (45a) and (51a) in comparison. In more detail, in figure the dashed (red) curve arises from Eq. (45a), and the solid (blue) curve arises from Eq. (51a). Data caption: $t = 0.5$; $\alpha = \beta = 1$; $T^\bullet = 1$; $\text{Kn} = 1$. The jump discontinuity therein occurs at the front of the moving temperature wave.

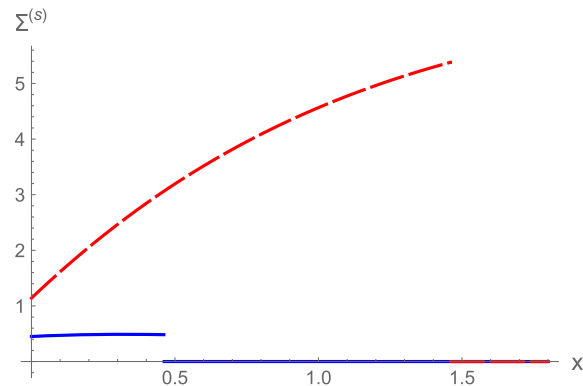


Fig. 6 $\Sigma^{(s)}$ versus x : analytical solutions arising from Eqs. (49b) and (52b) in comparison. In more detail, in figure the dashed (red) curve arises from Eq. (49b), and the solid (blue) curve arises from Eq. (52b). Data caption: $t = 0.8$; $\alpha = \beta = 1$; $T^\bullet = 1$; $\text{Kn} = 1$. The jump discontinuity therein occurs at the front of the moving temperature wave.

In the MC-theory the dimensionless 1D specific-entropy flux and production, respectively, read

$$G_x^{(s)} = \frac{h_x}{1 + T} \tag{52a}$$

$$\Sigma^{(s)} = - \frac{h_x}{(1 + T)^2} (\partial_x T + \partial_t h_x) \tag{52b}$$

In Figs. 6 and 7, we compare, instead, the behaviors of the analytical solutions by Eqs. (49b) and (52b) when $t = 0.8$, $\alpha = \beta = 1$, $T^\bullet = 1$, and $\text{Kn} = 1$ just for the sake of computation. From that figures, it follows that both the predicted specific-entropy productions tend to a plateau limit which is attained before the front of the moving temperature wave.

4 Final comments and future perspectives

The raise of nanotechnology has required (and, indeed, is still requiring) several efforts to better understand the thermal-transport properties of nanodevices, the performance and reliability of which could be much influenced by relaxation (i.e., memory), non-local and non-linear effects [2,7,33–35]. For this reason, in Eqs. (31) of this paper we proposed a non-linear and non-local thermodynamical model of heat transfer at nanoscale in a rigid body beyond the usual classical theories. That theoretical model, which encompasses both the F-theory, and the MC-theory as special cases, has been derived in framework of EIT [2,7] in Sect. 2 and essentially lies on the concept of flux of the heat flux Q_{ij} (which has been indeed decoupled into its deviatoric and bulk parts), the physical root of which arises from the kinetic theory [2].

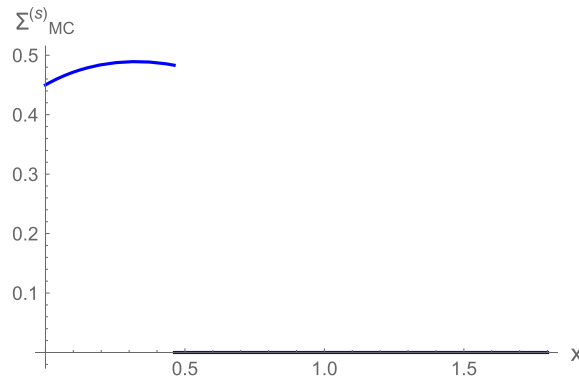


Fig. 7 $\Sigma^{(s)}$ versus x in the MC-case: detail of the qualitative behavior described in Fig. 6, i.e., analytical solution arising from Eq. (52b). Data caption: $t = 0.8$; $T^\bullet = 1$; $\text{Kn} = 1$. The jump discontinuity occurs at the front of the moving temperature wave.

Since in the present paper we derived Eqs. (31) only by means of macroscopic theoretical considerations, further comments about those equations are therefore needed. Besides to the form of the specific-entropy flux in Eq. (21), the theoretical model in Eqs. (31) is indeed also strictly related to Eq. (23) which substantially displays the bilinear form (24) in fluxes and forces. Although experimental observations confirm that thermodynamic forces and fluxes are interwoven [1,2], the exact relations among them are indeed not known a priori. In our approach we considered linear force-flux relations and, therefore, we finally set Eqs. (25). Non-linear flux-force relations could have been also considered in principle [36–39], indeed, in such a way that a different non-linear and non-local model of heat transfer was obtained. In the present paper, however, we did not pursue the approach of non-linear flux-force relations since it is generally related to theoretical questions concerning the interpretation of the second law (see Part I—Sec. 2.4 in Ref. [2], for example) which are surely conceptually interesting, but not properly in the focus of this paper.

By means of the so-called non-equilibrium-temperature approximation (i.e., whenever the difference $\theta^{-1} - \theta_{\text{eq}}^{-1} \rightarrow 0$), in Sect. 3 the non-linear terms in Eqs. (31) have been neglected and the propagation of thermal pulses in 1D nanosystems has been consequently analyzed. That analysis, although simplified, could be however useful in practical applications. For example, in current days the very high circuit densities yield modern chips run so hot that heat is becoming one of the major problems in the design of integrated circuits. As a consequence, one of the aspects which is much being studied at nanoscale is the isolation of very small areas which could be heated by an external source (either static as a hot spot due to a very miniaturized working device, or dynamic as a fast laser pulse): a continuous control of the temperature's rise, in fact, could be a crucial point for the correct operation of modern devices. In Sect. 3 we have tried to exactly tackle with that problem in 1D nanosystems. The analysis performed therein points out that one should pay attention to the role played by relaxation and non-local effects: as it follows from Fig. 2 (for the relaxation effects) and Fig. 3 (for the non-local effects) they may strongly influence the dissipative effects (i.e., one of the main—natural—tool for heat isolation of different components on a chip), thus not ensuring the right setting-up of modern devices which currently remains a very compelling challenge. That challenge could be also complicated by non-linear effects which may either enhance, or reduce, the influence of memory and non-local effects [15].

Another step toward a more detailed investigation will be surely the analysis of a pulse propagation once in Eqs. (31) no terms are neglected, or when non-linear flux-force relations are considered. We note that if Eqs. (31) are considered in their complete version, the interesting problem of flux limiters [22–24] also comes out: in that case, in fact, the form of the unknown fields will have to however guarantee that the effective thermal conductivity in Eq. (29) is positive defined.

The analysis performed in Sect. 3 could be, indeed, also used to indirectly compute a first rough estimation of the relaxation times of the high-order fluxes: whereas different models have been developed in order to estimate τ_R , very scant information about τ_1 and τ_0 (i.e., information on τ_N according with the observations in Sect. 2.2) can be found in the literature. Since the wave front depends on the ratios between those relaxation times and τ_R , as Fig. 2 clearly shows, by checking the wave front in practical applications one could also estimate whether τ_1 and τ_0 are larger (or smaller) than τ_R , in principle, for example.

At the very end, it seems worth noticing that, in general, it is not so simple to claim which is the best (or, alternatively said, the right) proposal among the different theories beyond the F-law. To this end, practical applications in which different theories clearly predict different results could be suitable benchmarks. This is,

for example, just the case of the heat-wave propagation we analyzed in the present paper: in fact, the results contained in Sect. 3 can be used to check, between the MC-theory and the model given by Eqs. (31), which one better fits with experimental evidences.

Acknowledgements The authors acknowledge Professor Francesco Oliveri from the University of Messina for fruitful discussions about this work which has been carried out under the auspices of the GNFM (Italian *National Group of Mathematical Physics*, INdAM).

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

Funding Open access funding provided by Università degli Studi di Salerno within the CRUI-CARE Agreement.

Appendix

At the end of this paper, just for the sake of completeness, we give some details about the technique used to solve the above IBVPs, the corresponding results of which are contained in Sect. 3.2.

Analytical solution

By applying the (temporal) Laplace transform $\mathcal{L}[\cdot]$ and recalling the usual relation

$$\mathcal{L}[\partial_t F(\mathbf{x}, t)](\nu) = \nu \mathcal{L}[F(\mathbf{x}, t)](\nu) - F_0(\mathbf{x}),$$

being ν the (complex) Laplace transform parameter and with $F_0(\mathbf{x}) = \lim_{t \rightarrow 0^+} F(\mathbf{x}, t)$, from Eqs. (42) we have the following system of ODEs

$$3\nu \mathcal{L}[\mathbf{T}] + \text{Kn}^2 d_x \mathcal{L}[\mathbf{h}_x] = 0 \quad (53a)$$

$$\alpha\beta(1+\nu) \mathcal{L}[\mathbf{h}_x] + \alpha\beta d_x \mathcal{L}[\mathbf{T}] + \alpha d_x \mathcal{L}\left[\overset{\circ}{\mathbf{H}}_{xx}\right] + \beta d_x \mathcal{L}[\mathbf{H}] = 0 \quad (53b)$$

$$3(1+\beta\nu) \mathcal{L}\left[\overset{\circ}{\mathbf{H}}_{xx}\right] + 4\beta \text{Kn}^2 d_x \mathcal{L}[\mathbf{h}_x] = 0 \quad (53c)$$

$$3(1+\alpha\nu) \mathcal{L}[\mathbf{H}] + 5\alpha \text{Kn}^2 d_x \mathcal{L}[\mathbf{h}_x] = 0 \quad (53d)$$

once the ID arising from the Laplace transform of Eqs. (43) have been employed in such a way they are *embedded* in the procedure. In the Laplace domain, moreover, the following BCs, arising from Eq. (44), have to be appended to Eqs. (53)

$$\mathcal{L}[\mathbf{T}](0, \nu) = \frac{\mathbf{T}^\bullet}{\nu} \quad \mathcal{L}[\mathbf{T}](+\infty, \nu) = 0 \quad (54)$$

Since Eqs. (53) substantially constitute a system of linear equations, by coupling Eq. (53a) with the spatial derivatives of Eqs. (53b)–(53d), we may obtain the following second-order ODE (in the unknown Laplace transform $\mathcal{L}[\mathbf{T}]$)

$$d_x^2 \mathcal{L}[\mathbf{T}] - \frac{\Omega^2}{\text{Kn}^2} \mathcal{L}[\mathbf{T}] = 0 \quad (55)$$

wherein we set

$$\Omega^2 = \frac{3\nu(1+\nu)(1+\alpha\nu)(1+\beta\nu)}{(\alpha\beta+4\alpha+5\beta)(\nu-\xi_1)(\nu-\xi_2)} \quad (56)$$

with

$$\xi_{1,2} = -\frac{\alpha+\beta+9 \mp \sqrt{(\alpha-\beta+1)^2+80}}{2(\alpha\beta+4\alpha+5\beta)} \quad (57)$$

just for the sake of a compact notation. Since the characteristic equation of ODE (55) is

$$\Lambda^2 = \frac{\Omega^2}{\text{Kn}^2} \quad (58)$$

by means of BCs in Eq. (54) we are led to

$$\mathcal{L}[\mathbf{T}] = \left(\frac{\mathbf{T}^\bullet}{\nu}\right) e^{-\frac{\Omega}{\text{Kn}}x} \quad (59)$$

which reduces to

$$\mathcal{L}[\mathbf{T}] = \left(\frac{\mathbf{T}^\bullet}{\nu}\right) e^{-\frac{\xi}{\text{Kn}}(\nu+\epsilon)x} \quad (60)$$

once infinitesimals of order lower than ν^{-1} have been neglected in computing Ω (i.e., when the square root of Eqs. (56) is evaluated), and Eq. (46) hold. Considerations about the degree of the above approximation can be found in the second section of this appendix.

From Eqs. (53) we may straightforwardly have

$$\mathcal{L}[\mathbf{h}_x] = \left(\frac{3\mathbf{T}^\bullet}{\xi \text{Kn} \nu}\right) \left(1 - \frac{\epsilon}{\nu}\right) e^{-\frac{\xi}{\text{Kn}}(\nu+\epsilon)x} \quad (61a)$$

$$\mathcal{L}\left[\overset{\circ}{\mathbf{H}}_{xx}\right] = \left(\frac{4\beta\mathbf{T}^\bullet}{1+\beta\nu}\right) e^{-\frac{\xi}{\text{Kn}}(\nu+\epsilon)x} \quad (61b)$$

$$\mathcal{L}[\mathbf{H}] = \left(\frac{5\alpha\mathbf{T}^\bullet}{1+\alpha\nu}\right) e^{-\frac{\xi}{\text{Kn}}(\nu+\epsilon)x}. \quad (61c)$$

The inverse (temporal) Laplace transforms of Eqs. (60) and (61) furnish Eqs. (45).

In the MC-theory Eqs. (50) holds; therefore in the Laplace domain one has

$$3\nu\mathcal{L}[\mathbf{T}] + \text{Kn}^2 d_x\mathcal{L}[\mathbf{h}_x] = 0 \quad (62a)$$

$$(1+\nu)\mathcal{L}[\mathbf{h}_x] + d_x\mathcal{L}[\mathbf{T}] = 0 \quad (62b)$$

which leads to

$$\mathcal{L}[\mathbf{T}] = \left(\frac{\mathbf{T}^\bullet}{\nu}\right) e^{-\frac{\sqrt{3}}{\text{Kn}}(\nu+\frac{1}{2})x} \quad (63a)$$

$$\mathcal{L}[\mathbf{h}_x] = \left(\frac{\sqrt{3}\mathbf{T}^\bullet}{\text{Kn} \nu}\right) \left(1 - \frac{1}{2\nu}\right) e^{-\frac{\sqrt{3}}{\text{Kn}}(\nu+\frac{1}{2})x} \quad (63b)$$

once the BCs in Eqs. (54) is employed. The inverse (temporal) Laplace transforms of Eqs. (63) give Eqs. (51).

Numerical solution

Although we refer to Eqs. (45) as the analytical solution of the IBVP in Eqs. (42)–(44), it seems worth noticing that they are not exact solutions since we neglected infinitesimals of order lower than ν^{-1} in deriving Eq. (60). The small-time approximation is surely logical in very fast phenomena (as the pulse propagation at hand), but *a priori* the orders of infinitesimals which may be neglected are not known.

To be sure that the approximation we used does not significantly affect Eqs. (45), we also perform a comparison with a numerical solution. In Fig. 8, we show how effective is the approximation used to obtain the analytical expression for the temperature field in Eq. (45a) (which is fundamentally the real benchmark in the present approach). In particular therein the solid (blue) curve refers to Eq. (45a), whereas the dotted (red) curve has been obtained by inverting numerically the exact Laplace transform of the temperature field

$$\mathcal{L}[\mathbf{T}] = \frac{\mathbf{T}^\bullet}{\nu} e^{-\frac{\Omega}{\text{Kn}}x} \quad (64)$$

through the modified Tzou series [40]

$$\mathcal{F}(x, t) \approx \frac{e^{4.7}}{t} \left\{ \frac{1}{2} \mathcal{L}[\mathcal{F}] \left(x, \frac{4.7}{t}\right) + \text{Re} \left[\sum_{j=1}^M (-1)^j \mathcal{L}[\mathcal{F}] \left(x, \frac{4.7 + ij\pi}{t}\right) \text{sinc} \left(\frac{j\pi}{M}\right) \right] \right\} \quad (65)$$

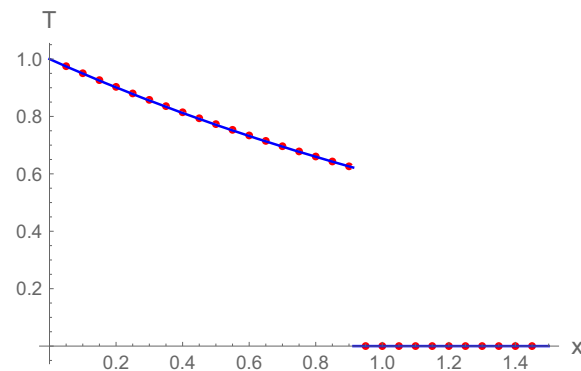


Fig. 8 T versus x : (approximate) analytical solution (solid line) in comparison with (exact) numerical solution (dotted line). Data caption: $t = 0.5$; $\alpha = \beta = 1$; $T^* = 1$; $Kn = 1$

for $M = 500$, with Ω given by Eq. (56).

The very good agreement between the two solutions in Fig. 8 (obtained also for data captions different from those used in that figure) ensures that the aforementioned approximation plays no relevant role in Eqs. (45).

References

- De Groot, S.R., Mazur, P.: Non-equilibrium Thermodynamics. North-Holland Publishing Company, Amsterdam (1962)
- Jou, D., Casas-Vázquez, J., Lebon, G.: Extended Irreversible Thermodynamics, 4th edn. Springer, Berlin (2010)
- Muschik, W., Ehrentauf, H.: An amendment to the Second Law. *J. Non-Equilib. Thermodyn.* **21**, 175–192 (1996)
- Jou, D., Lebon, G., Mongiovi, M.S., Peruzza, R.A.: Entropy flux in non-equilibrium thermodynamics. *Physica A* **338**, 445–457 (2004)
- Sellitto, A., Cimmelli, V.A., Jou, D.: Entropy flux and anomalous axial heat transport at the nanoscale. *Phys. Rev. B* **87**, 054302 (2013)
- Chowdhury, S.C., Roy, D., Reddy, J.N.: Relating entropy flux with heat flux in two-temperature thermodynamic model for metal thermoviscoplasticity. *J. Appl. Mech.* **84**, 021007 (2017)
- Lebon, G., Jou, D., Casas-Vázquez, J.: Understanding Non-equilibrium Thermodynamics. Springer, Berlin (2008)
- Cimmelli, V.A., Sellitto, A., Jou, D.: Nonequilibrium temperatures, heat waves, and nonlinear heat transport equations. *Phys. Rev. B* **81**, 054301 (2010)
- Uribe, F.J.: Shock waves: the Maxwell-Cattaneo case. *Phys. Rev. E* **93**, 033110 (2016)
- Hennesy, M.G., Calvo-Schwarzwälder, M., Myers, T.G.: Modelling ultra-fast nanoparticle melting with the Maxwell-Cattaneo equation. *Appl. Math. Model.* **69**, 201–222 (2019)
- Herrera, L., Pávon, D.: Hyperbolic theories of dissipation: Why and when do we need them? *Physica A* **307**, 121–130 (2002)
- Cattaneo, C.: Sulla conduzione del calore. *Atti Sem. Mat. Fis. Univ. Modena* **3**, 83–101 (1948)
- Guo, Y., Wang, M.: Phonon hydrodynamics and its applications in nanoscale heat transport. *Phys. Rep.* **595**, 1–44 (2015)
- Guyer, R.A., Krumhansl, J.A.: Solution of the linearized phonon Boltzmann equation. *Phys. Rev.* **148**, 766–778 (1966)
- Sellitto, A., Cimmelli, V.A., Jou, D.: Analysis of three nonlinear effects in a continuum approach to heat transport in nanosystems. *Physica D* **241**, 1344–1350 (2012)
- Di Domenico, M., Jou, D., Sellitto, A.: Nonlocal and nonlinear contributions to the thermal and elastic high-frequency wave propagations at nanoscale. *Int. J. Heat Mass Transf.* **156**, 119888 (2020)
- Di Domenico, M., Jou, D., Sellitto, A.: Heat-flux dependence of the speed of nonlinear heat waves: Analogies with the Kerr effect in nonlinear optics. *Int. J. Therm. Sci.* **161**, 106719 (2021)
- Dong, Y., Cao, B.-Y., Guo, Z.-Y.: Generalized heat conduction laws based on thermomass theory and phonon hydrodynamics. *J. Appl. Phys.* **110**, 063504 (2011)
- Lebon, G., Torrisi, M., Valenti, A.: A non-local thermodynamic analysis of second sound propagation in crystalline dielectrics. *J. Phys. Condens. Matter* **7**, 1461–1474 (1997)
- Carlomagno, I., Di Domenico, M., Sellitto, A.: High-order fluxes in heat transfer with phonons and electrons: Application to wave propagation. *Proc. R. Soc. A* **477**, 20210392 (2021)
- Kovács, R., Madjarević, D., Simić, S., Ván, P.: Non-equilibrium theories of rarefied gases: internal variables and extended thermodynamics. *Contin. Mech. Thermodyn.* **33**, 307–325 (2021)
- Levermore, C.D.: Relating Eddington factors to flux limiters. *J. Quant. Spec. Rad. Transf.* **31**, 149–160 (1984)
- Anile, A.M., Romano, V.: Covariant flux-limited diffusion theories. *Astrophys. J.* **386**, 325–329 (1992)
- Sellitto, A., Cimmelli, V.A.: Flux limiters in radial heat transport in silicon nanolayers. *J. Heat Transf. Trans. ASME* **136**, 071301 (2014)
- Dreyer, W., Struchtrup, H.: Heat pulse experiments revisited. *Contin. Mech. Thermodyn.* **5**, 3–50 (1993)
- Ziman, J.M.: Electrons and Phonons. Oxford University Press, Oxford (2001)
- Chen, R., Hochbaum, A.I., Murphy, P., Moore, J., Yang, P., Majumdar, A.: Thermal conductance of thin silicon nanowires. *Phys. Rev. Lett.* **101**, 105501 (2008)

28. Cahill, D.G., Braun, P.V., Chen, G., Clarke, D.R., Fan, S., Goodson, K.E., Keblinski, P., King, W.P., Mahan, G.D., Majumdar, A., Maris, H.J., Phillpot, S.R., Pop, E., Shi, L.: Nanoscale thermal transport II. 2003–2012. *Appl. Phys. Rev.* **1**(1), 011305 (2014)
29. Struchtrup, H., Öttinger, H.C.: Thermodynamically admissible 13-moment equations. *Phys. Fluid* **34**, 017105 (2022)
30. Grad, H.: On the kinetic theory of rarefied gases. *Commun. Pure Appl. Math.* **2**, 331–407 (1949)
31. Grmela, M., Öttinger, H.: Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. *Phys. Rev. E* **56**(6), 6620–6632 (1997)
32. Sellitto, A., Di Domenico, M.: Nonlocal and nonlinear contributions to the thermal and elastic high-frequency wave propagations at nanoscale. *Contin. Mech. Thermodyn.* **31**, 807–821 (2019)
33. Tzou, D.Y.: *Macro to Micro-scale Heat Transfer. The Lagging Behaviour*. Taylor and Francis, New York (1997)
34. Chen, G.: *Nanoscale Energy Transport and Conversion—A Parallel Treatment of Electrons, Molecules, Phonons, and Photons*. Oxford University Press, Oxford (2005)
35. Zhang, Z.M.: *Nano/Microscale Heat Transfer*. McGraw-Hill, New York (2007)
36. Hurley, J., Garrod, C.: Generalization of the Onsager reciprocity theorem. *Phys. Rev. Lett.* **48**, 1575–1577 (1982)
37. Verhás, J.: An extension of the governing principle of dissipative processes to nonlinear constitutive equations. *Ann. Phys.* **495**, 189–193 (1983)
38. Johannessen, E., Kjelstrup, S.: Nonlinear flux-force relations and equipartition theorems for the state of minimum entropy production. *J. Non-Equilib. Thermodyn.* **30**, 129–136 (2005)
39. Salazar, D.S.P., Landi, G.T.: Nonlinear Onsager relations for Gaussian quantum maps. *Phys. Rev. Res.* **2**, 033090 (2020)
40. Keiffer, R.S., Jordan, P.M., Christov, I.C.: Acoustic shock and acceleration waves in selected inhomogeneous fluids. *Mec. Res. Commun.* **93**, 80–88 (2018)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.