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# Heat transfer at nanoscale and boundary conditions

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**Abstract.** A model of nonlocal heat transfer at nanoscale in rigid bodies is considered. Depending on the relevance of the particular interaction's mechanism between the heat carriers and the lateral walls, three different strategies for the setting-up of the boundary conditions are analyzed, and the consequent forms of the basic fields have been obtained, as well. From the physical point of view, the possible influence of those interactions on the unknown fields is pointed out. From the mathematical point of view, instead, the well-posedness of the problem is shown.

**Mathematics Subject Classification.** 74A15, 35E15, 35Q79, 80A05.

**Keywords.** Nanoscale heat transfer, Phonon–wall interactions, Nonlocal effects, Boundary conditions.

## 1. Introduction

The rapid progress in nanotechnology and its very huge impact in modern life have stimulated a true revolution in the heat-transfer phenomenon, spreading its domain of applicability and discovering new regimes and phenomenologies wherein either the Fourier law, or classical (continuum thermodynamic) theories are no longer applicable, if one aims at the correct modeling and interpretation of the experimental data [1–11].

An outstanding model of heat transfer in a rigid body at nanoscale (which goes beyond the classical thermodynamics) lies upon the following equations [1,2,4,5]:

$$c_{\mathrm{v}}\dot{\theta} + q_{i,i} = 0 \tag{1a}$$

$$\tau\dot{q}_i + q_i + \kappa\theta_{,i} - \ell^2\left(2q_{j,ji} + q_{i,jj}\right) = 0 \tag{1b}$$

**Remark 1.** Throughout this paper, we assume that all fields are defined in a fixed and compact subset $\Omega \subset \mathbb{R}^3$ with a piecewise smooth boundary $\partial\Omega$. Since the arguments of the present study regard solid materials, we assume for $\Omega$ the mathematical model of a rigid body, i.e., the boundary $\partial\Omega$ is independent of time ($t$) here.

In the above theoretical model the heat transport in $\Omega$ is described by means of momentum and energy exchanges between phonons (i.e., quanta of the vibrational mechanical energy arising from oscillating atoms within a crystal which, in the present paper, are the only heat carriers). In more details, in Eq. (1) we have

$$\theta = T - T_0 \tag{2}$$

with $T$ being the non-equilibrium temperature [12,13], whereas $T_0$ is the (constant) reference value of the local-equilibrium temperature. In those equations, furthermore, $q_i$ means the local heat-flux vector, $c_{\mathrm{v}}$ the specific heat at constant volume (per unit volume), $\kappa$ the thermal conductivity, $\tau$ the relaxation time of resistive phonon collisions, and $\ell$ the phonon mean-free path (related both to the resistive, and to the normal phonon collisions).

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We note that Eq. (1a) directly follows from the local balance of energy in the case of a rigid body, once the usual relation $du = c_v dT$ ($u$ being the internal energy per unit volume) is used; Eq. (1b), instead, has been derived for the first time in Refs. [1,2] starting from the Boltzmann equation for phonons in the Callaway approximation [4,5]. The compatibility of Eqs. (1) with the basic tenets of Continuum Mechanics has been proved in different contexts (see § 9.3.2 in Ref. [5], for example). Further comments about Eq. (1b) are postponed in the closing section of this paper. The main merit of Eqs. (1) in the determination of the unknown basic fields $\theta$ (or, alternatively, $T$ by means of Eq. (2)) and $q_i$ is the emphasis given to the role of the nonlocal effects in the heat transport, a topic of much interest at nanoscale wherein even small temperature differences may lead to high temperature gradients.

From a pure mathematical point of view, one could indeed observe that the actual values of the aforementioned basic fields (predicted by Eqs. (1)) are strictly related to initial and boundary conditions (BCs), the setting-up of the latter primarily made in order to ensure a well-posed problem. From the physical point of view, instead, those conditions should arise from physical evidences and/or have a 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.

The right setting-up of BCs, instead, is more delicate and controversial. It should be noted, moreover, that in the case of Eqs. (1) it becomes still more acute since therein the two unknown fields are coupled: the BCs on $\theta$ and $q_i$, therefore, cannot be independent of each other. As a consequence, the following question may naturally arise: how to correctly furnish BCs to solve Eqs. (1) both from the physical, and from the mathematical point of view? To answer that question one may follow different strategies, and/or theoretical models [5,14–18].

Especially focusing our attention on the role played by the heat flux in the BCs setting-up, from the pure mathematical point of view here we propose and investigate three possible strategies that can be used to tackle Eqs. (1). As it will be discussed in what follows, those strategies, which may be related both to the particular heat-transport regime and to the wall features, have also a clear physical root in such a way that two of them represent special cases which can be found, in principle, in practical applications at nanoscale in dealing with the propagation of heat. The present study, therefore, aims at a complete analysis of heat transfer at nanoscale: without loss of continuity, in fact, by means of our proposal one might correctly describe a very wide range of heat-transfer regime. In the special case of one-dimensional (1D) heat transfer, in particular, the goal of this paper is twofold:

(i) From the mathematical point of view, we prove existence and uniqueness of the basic fields in all the aforementioned BC strategies;
(ii) From the physical point of view, we try to point out the possible (relevant) influence of phonon–wall interactions on the form of the basic fields.

Summarizing, the present article is organized as follows:

- In Sect. 2 we write down the 1D model equations arising from Eqs. (1);
- In Sect. 3 we investigate about the existence and uniqueness of the solutions of different boundary value problems related to Eqs. (1);
- In Sect. 4 we furnish the solutions of Eqs. (1) in the above cases of BCs, and comment about the possible relevance of the phonon–wall interactions;
- in Sec 5 we give final remarks and comments.

## 2. Heat transfer in 1D nanostructures

In this paper, we are primarily interested in thermal transport within the so-called 1D nanostructures (specifically nanowires, nanofibers, nanotubes, and nanorods). For some comprehensive reviews about the use of these material systems, the readers can refer, for example, to Refs. [19,20] and the references cited therein. Here we however note that the use of 1D nanostructured materials (with compositions based on oxides, nitrides, or metals) either due to an extraordinary surface-volume relationship, or to tunable thermal and transport properties, have become fundamental elements for the development of energy processes. The heat transfer has been also studied in 1D multi-layer models of polymer foams in order to determine the equivalent thermal conductivity [21].

In the present analysis, therefore, we always have $\Omega \equiv [0, l]$ and $\partial\Omega \equiv \{0; l\}$, $l$ being the characteristic (finite) length of the system at hand. Specifically, in what follows we assume 1D heat flow along the $z$-axis of a Cartesian coordinate system (see Fig. 1 for a qualitative sketch of the coordinate system under consideration in the present paper, for example). In this case the aforementioned unknown fields take the forms

$$\theta = \theta\,(x, t) \tag{3a}$$

$$q_i = (q\,(x, t)\,; 0; 0) \tag{3b}$$

and, consequently, Eq. (1) reduces to

$$c_{\mathrm{v}}\theta_t + q_x = 0 \tag{4a}$$

$$\tau q_t + q + \kappa\theta_x - 3\ell^2 q_{xx} = 0 \tag{4b}$$

**Notation 1.** *From now on, a subscript $t$ denotes time partial derivatives (i.e., $f_t := \frac{\partial f}{\partial t}$), and a subscript $x$ stands for spatial partial derivative (i.e., $f_x := \frac{\partial f}{\partial x}$).*

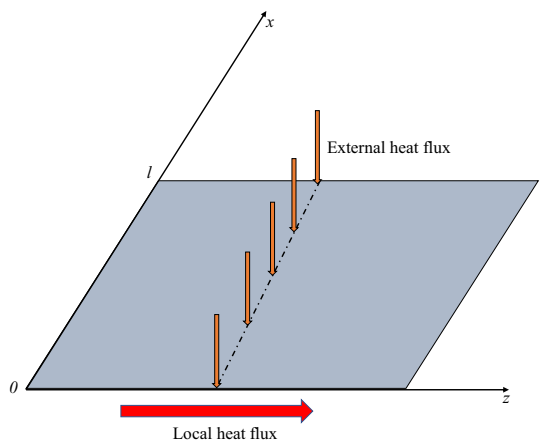


FIG. 1. Nanolayer heated by an external heat flux perpendicular to it (i.e., the vertical arrows—orange in figure) which produces a heat flux (i.e., the horizontal arrow—red in figure) in the longitudinal $z$ direction. In this case the subset $\Omega$ indicates a transversal section (i.e., the dashed-dotted line, sketched in figure, the length of which is $l$) of the nanolayer which becomes the interval $[0; 1]$ once the non-dimensional variable $\mathsf{x}$ is introduced. The two fields $h\,(\mathsf{x}, \mathsf{t})$ and $\vartheta\,(\mathsf{x}, \mathsf{t})$ are, instead, the (non-dimensional) local heat flux and deviation of the non-equilibrium temperature from the local-equilibrium temperature in that transversal section, respectively (color figure online)

For computational convenience, we introduce the dimensionless variables

$$\mathsf{x} := \frac{x}{l} \quad \mathsf{t} := \frac{t}{\tau} \quad \vartheta := \frac{\theta}{T_0} \quad h := \frac{lq}{\kappa T_0} \tag{5}$$

such that we have $\Omega \equiv [0,1]$ and $\partial\Omega \equiv \{0;1\}$. Equations (5), indeed, also allows us to switch from the original couples of

- variables $(x,t) \in [0,l] \times [0,t_f)$ to the new couple of variables $(\mathsf{x},\mathsf{t}) \in [0,1] \times [0,\infty)$;
- unknown functions $\theta$ and $q$ to the new couple of unknown functions $\vartheta, h: \ [0,1] \times \ [0,\infty) \mapsto \mathbb{R}$.

Furthermore, if we estimate the resistive relaxation time of phonons as

$$\tau = \frac{\ell}{\mathrm{V}_{0\mathrm{p}}} \tag{6}$$

wherein $\mathrm{V}_{0\mathrm{p}}$ stands for the average phonon speed (measured at the reference temperature-value $T_0$), and we use the well-known *Ziman limit* [22] for the thermal conductivity, i.e., if we assume that

$$\kappa = \frac{c_{\mathrm{v}} \tau \mathrm{V}_{0\mathrm{p}}^2}{3} \tag{7}$$

then straightforward calculations may show that Eqs. (4) becomes

$$\vartheta_{\mathsf{t}} + \frac{\mathrm{Kn}^2}{3} h_{\mathsf{x}} = 0 \tag{8a}$$

$$h_{\mathsf{t}} + h + \vartheta_{\mathsf{x}} - 3\mathrm{Kn}^2 h_{\mathsf{xx}} = 0 \tag{8b}$$

with

$$\mathrm{Kn} = \frac{\ell}{l} \tag{9}$$

being the so-called *Knudsen number* of the heat transfer. We note that in the case of nanoscale (thermal) transport regimes one usually has $\mathrm{Kn} \sim \mathcal{O}(1)$ (i.e., $\ell \geq l$), whereas the cases in which $\mathrm{Kn} \to 0^+$ (i.e., $\ell \ll l$) correspond to macroscale (thermal) transport regimes.

**Remark 2.** Depending on the Kn value, in principle, at nanoscale the following three different heat-transfer regimes can be found [23,24]:

- Fourier diffusive regime. In this case Kn is small, and the phonons principally undergo multiple scattering in the bulk of the system.
- Poiseuille phonon flow. In this case Kn attains moderate values, and the phonon–wall collisions are comparable to the internal (i.e., in the bulk) phonon scatterings.
- Ballistic regime. In this case Kn is very high, and the boundary-phonon scattering becomes prevalent among the other mechanisms of scatterings.

Referring the readers to Sect. 3 for the theoretical models of BCs, it seems worth observing that to our goals we also need prescribing initial data (ID) for the two unknown scalar-valued functions $h$ and $\vartheta$, too. To this end, let us here assume

$$h(\mathsf{x},0) = h_0(\mathsf{x}), \quad \forall \mathsf{x} \in [0,1] \tag{10a}$$

$$\vartheta(\mathsf{x},0) = 0, \qquad \forall \mathsf{x} \in [0,1] \tag{10b}$$

wherein $h_0$ is a regular scalar-valued function of the indicated argument.

**Remark 3.** From the practical point of view, the above ID means that the system at hand is perturbed from its local equilibrium only by the application of an external heat flux, given by Eq. (10a). In Ref. [25] (see, in particular, therein § 4), for example, the authors proposed (externally controllable) heat lenses, namely, the possibility of focusing plane heat waves into a given (focal) point by the external application

of a heat flux in the orthogonal direction of a nanolayer. In that case, for example, $\Omega$ will be just a transversal section of the nanolayer (see Fig. 1 for a qualitative sketch) wherein the behaviors of the two unknown fields $h(\mathsf{x},\mathsf{t})$ and $\vartheta(\mathsf{x},\mathsf{t})$ have to be determined for own practical needs.

According with the observations made in Sect. 1, since in the next we choose to prescribe BCs on the unknown function $h(\mathsf{x},\mathsf{t})$, BCs on the unknown function $\vartheta(\mathsf{x},\mathsf{t})$ cannot be freely imposed, too, but they have to directly follow from the model equations. To this end, as a direct consequence of Eqs. (8a) and (10b), we may observe that we are able to write

$$\vartheta(\mathsf{x},\mathsf{t}) = -\frac{\mathrm{Kn}^2}{3}\int_0^{\mathsf{t}} h_{\mathsf{x}}(\mathsf{x},\mathcal{T})\mathrm{d}\mathcal{T} \tag{11}$$

and hence we have

$$\vartheta(0,\mathsf{t}) = -\frac{\mathrm{Kn}^2}{3}\int_0^{\mathsf{t}} h_{\mathsf{x}}(0,\mathcal{T})\mathrm{d}\mathcal{T}, \quad \forall \mathsf{t}\in\mathbb{R}^+ \tag{12a}$$

$$\vartheta(1,\mathsf{t}) = -\frac{\mathrm{Kn}^2}{3}\int_0^{\mathsf{t}} h_{\mathsf{x}}(1,\mathcal{T})\mathrm{d}\mathcal{T}, \quad \forall \mathsf{t}\in\mathbb{R}^+ \tag{12b}$$

as the BCs for the unknown scalar-valued function $\vartheta(\mathsf{x},\mathsf{t})$.

## 3. BCs setting-up: existence and uniqueness of solutions

The aim of this section is to prove the well-posedness of the proposed problem. To this end, we will use the semigroup of linear operators theory. The first step is to see our problem as an abstract Cauchy problem defined on a convenient Hilbert space. Precisely we will prove existence and uniqueness of the solutions of our model equations by appending to Eqs. (1) three different types of BCs for the local heat-flux field and, investigating the consequent problems principally from the mathematical point of view, we recast Eqs. (8) into an abstract setting introducing a suitable functional framework. Some physical considerations about the above BCs setting-up strategies are given in Sect. 5.

Let's consider, therefore, the functional space

$$\mathcal{H} = L^2(0,1)\times L^2(0,1) \tag{13}$$

and let $\mathcal{A}$ be the operator given by

$$\mathcal{A}\mathbf{U} = \begin{pmatrix} -h(\mathsf{x},\mathsf{t}) - \vartheta_{\mathsf{x}}(\mathsf{x},\mathsf{t}) + 3\mathrm{Kn}^2 h_{\mathsf{xx}}(\mathsf{x},\mathsf{t}) \\ -\dfrac{\mathrm{Kn}^2}{3} h_{\mathsf{x}}(\mathsf{x},\mathsf{t}) \end{pmatrix} \tag{14}$$

where $\mathbf{U} = (h,\vartheta)\in\mathcal{H}$.

### 3.1. Strategy I: the Robin BCs

In order to solve Eqs. (1) the following Robin (R-) type BCs can be used:

$$q_i - C\ell q_{i,j} n_j = 0, \quad \forall x_i \in \partial\Omega,\ \forall t \geq 0 \tag{15}$$

Equation (15), with $n_j$ meaning the outward normal-unit vector to $\partial\Omega$, states that in principle the local heat flux attains a non-vanishing value at the walls: for this reason we also use the appellation *slip-heat* BCs when we refer to Eq. (15). Moreover, therein $C$ is a positive constant (non-dimensional) parameter which can be related to boundary's features and models the phonon–wall interactions. Although other

theoretical proposals of BCs for $q_i$ can be found in literature (see, for example, Ref. [26]), avoiding a deeper microscopic derivation of Eq. (15), let us here only note that they are similar to the velocity-slip condition in the so-called Maxwell-slip model for rarefied gases [27–29]. A heuristic derivation of Eq. (15) can be also found in Ref. [17] (see therein § 5). Further physical considerations about Eq. (15) (especially on $C$) are postponed to Sect. 5.

In 1D situations Eq. (15) yields

$$h(0,\mathsf{t}) - C\mathrm{Kn}h_{\mathsf{x}}(0,\mathsf{t}) = 0, \quad \forall \mathsf{t} \in \mathbb{R}^+ \tag{16a}$$

$$h(1,\mathsf{t}) + C\mathrm{Kn}h_{\mathsf{x}}(1,\mathsf{t}) = 0, \quad \forall \mathsf{t} \in \mathbb{R}^+ \tag{16b}$$

when the dimensionless variables in Eq. (5) are introduced. Once the R-BCs in Eqs. (16) hold, $\mathcal{H}$ in Eq. (13) is a Hilbert space with the norm

$$\|\mathbf{U}\|_{\mathcal{H}}^2 = \|h\|^2 + \frac{3}{\mathrm{Kn}^2}\|\vartheta\|^2 + \frac{3C}{\mathrm{Kn}}\left[|\vartheta(0,\mathsf{t})|^2 + |\vartheta(1,\mathsf{t})|^2\right] . \tag{17}$$

In addition, the domain $D(\mathcal{A})$ of the operator defined in Eq. (14) is

$$D(\mathcal{A}) = \left\{ \begin{array}{c} \mathbf{U} \in \mathcal{H}; \quad h \in H^2(0,1), \vartheta \in H^1(0,1): \\ h(0,\mathsf{t}) = C\mathrm{Kn}h_{\mathsf{x}}(0,\mathsf{t}) \qquad \text{and} \qquad h(1,\mathsf{t}) = -C\mathrm{Kn}h_{\mathsf{x}}(1,\mathsf{t}) \\ \vartheta(0,\mathsf{t}) = -\frac{\mathrm{Kn}^2}{3}\int_0^{\mathsf{t}} h_{\mathsf{x}}(0,\mathcal{T})\mathrm{d}\mathcal{T} \text{ and } \vartheta(1,\mathsf{t}) = -\frac{\mathrm{Kn}^2}{3}\int_0^{\mathsf{t}} h_{\mathsf{x}}(1,\mathcal{T})\mathrm{d}\mathcal{T} \end{array} \right\}$$

Under the above notations, the original problem can be therefore written as

$$\frac{\mathrm{d}}{\mathrm{d}\mathsf{t}}\mathbf{U}(\mathsf{t}) = \mathcal{A}\mathbf{U}(\mathsf{t}), \quad \mathbf{U}(0) = \mathbf{U}_0, \quad \forall \mathsf{t} \in \mathbb{R}^+ \tag{18}$$

wherein $\mathbf{U}_0 \in \mathcal{H}$ stands for the initial datum defined by Eqs. (10).

The well-posedness of the problem given above is guaranteed by the following results.

**Theorem 1.** *Let the operator $\mathcal{A}$ be given by Eq. (14). Then $\mathcal{A}$ generates a $C_0$-semigroup $\mathcal{G}(\mathsf{t})$ of contractions over $\mathcal{H}$.*

*Proof.* First of all, $D(\mathcal{A})$ is dense in $\mathcal{H}$ and it is straightforward to prove that $0 \in \varrho(\mathcal{A})$ (the resolvent set of $\mathcal{A}$). To this aim, suppose that $0 \notin \varrho(\mathcal{A})$; therefore there exists $\mathbf{U} \neq 0$ in $D(\mathcal{A})$ satisfying equation $\mathcal{A}\mathbf{U} = 0$ which, in terms of its components, can be explicitly written as

$$-h(\mathsf{x},\mathsf{t}) - \vartheta_{\mathsf{x}}(\mathsf{x},\mathsf{t}) + 3\mathrm{Kn}^2 h_{\mathsf{xx}}(\mathsf{x},\mathsf{t}) = 0 \tag{19a}$$

$$-\frac{\mathrm{Kn}^2}{3}h_{\mathsf{x}}(\mathsf{x},\mathsf{t}) = 0 \tag{19b}$$

From Eq. (19b) it follows $h_{\mathsf{x}}(\mathsf{x},\mathsf{t}) = 0$, which implies $h(\mathsf{x},\mathsf{t}) = 0$ because, from Eqs. (16), $h$ becomes a null function on the boundary. Substituting this into Eq. (19a), it follows that $\vartheta_{\mathsf{x}}(\mathsf{x},\mathsf{t}) = 0$. Since Eqs. (12) assures that also $\vartheta$ becomes a null function on the boundary, we conclude that $\vartheta = 0$. This shows that $\mathbf{U} = 0$, which is a contradiction. Therefore, $0 \in \varrho(\mathcal{A})$.

In addition it is not difficult to see that $\mathcal{A}$ is a dissipative operator in the space $\mathcal{H}$. More precisely, multiplying Eq. (8a) and Eq. (8b) by $h$ and $\vartheta$, respectively, integrating by part and using boundary conditions, we have that the Real part of the corresponding scalar product in $\mathcal{H}$ can be written as

$$\mathrm{Re}\langle\mathcal{A}\mathbf{U}, \mathbf{U}\rangle_{\mathcal{H}} = -\left[\|h\|^2 + 3\mathrm{Kn}^2\|h_{\mathsf{x}}\|^2 + 3C\mathrm{Kn}^3\left(|h_{\mathsf{x}}(0,\mathsf{t})|^2 + |h_{\mathsf{x}}(1,\mathsf{t})|^2\right)\right] \tag{20}$$

Therefore, from Lumer–Phillip's theorem (see Ref. [30]), we have that $\mathcal{A}$ is the infinitesimal generator of a contraction $C_0$-semigroup □

From Theorem 1 we can then state the following result (see Ref. [30]):

**Theorem 2.** (Existence and Uniqueness) *For any* $\mathbf{U}_0 \in \mathcal{H}$ *there exists a unique mild solution of the problem set by Eq.* (18). *Moreover, if* $\mathbf{U}_0 \in D(\mathcal{A})$ *then the solution is strong and* $\mathbf{U} \in C^1([0,\infty);\mathcal{H}) \cap C([0,\infty);D(\mathcal{A}))$.

According to Theorems 1 and 2, for a given initial datum $\mathbf{U}_0 \in \mathcal{H}$ we have

$$\mathbf{U}(\mathsf{t}) = \mathcal{G}(\mathsf{t})\,\mathbf{U}_0$$

### 3.2. Strategy II: the Dirichlet BCs

Equations (1) can be also solved by means of the following Dirichlet (D-) type BCs for the local heat-flux field:

$$q_i = 0, \quad \forall x_i \in \partial\Omega,\ \forall t \geq 0 \tag{21}$$

Equation (21), which state that the local heat flux attains a vanishing value at the walls, in 1D situations becomes

$$h(0,\mathsf{t}) = 0, \quad \forall \mathsf{t} \in \mathbb{R}^+ \tag{22a}$$

$$h(1,\mathsf{t}) = 0, \quad \forall \mathsf{t} \in \mathbb{R}^+ \tag{22b}$$

when the dimensionless variables in Eqs. (5) are introduced. We note that the D-BCs in Eq. (21) (or, alternatively, in Eqs. (22)) directly arise from the R-BCs in Eq. (15) (or, alternatively, in Eqs. (16)) when $C \to 0^+$, namely, when the diffusive phonon–wall scatterings are predominant. For this reason, we also use the appellation *diffusive* BCs when we refer to Eqs. (22).

The well-posedness of our problem is guaranteed if we consider D-BCs, too. In this case, the domain of the operator $\mathcal{A}$ defined in Eq. (14) becomes

$$D(\mathcal{A}) = \left\{ \begin{array}{c} \mathbf{U} \in \mathcal{H}; \quad h \in H_0^2(0,1), \vartheta \in H^1(0,1): \\ \vartheta(0,\mathsf{t}) = -\frac{\mathrm{Kn}^2}{3}\int_0^{\mathsf{t}} h_{\mathsf{x}}(0,\mathcal{T})\mathrm{d}\mathcal{T} \text{ and } \vartheta(1,\mathsf{t}) = -\frac{\mathrm{Kn}^2}{3}\int_0^{\mathsf{t}} h_{\mathsf{x}}(1,\mathcal{T})\mathrm{d}\mathcal{T} \end{array} \right\}$$

and its norm and dissipativeness can be obtained by Eqs. (17) and (20), respectively, by imposing $C \to 0^+$. In fact they read

$$\|\mathbf{U}\|_{\mathcal{H}}^2 = \|h\|^2 + \frac{3}{\mathrm{Kn}^2}\|\vartheta\|^2 \tag{23}$$

and

$$\mathrm{Re}\langle \mathcal{A}\mathbf{U}, \mathbf{U}\rangle_{\mathcal{H}} = -\left[\|h\|^2 + 3\mathrm{Kn}^2\|h_{\mathsf{x}}\|^2\right] \tag{24}$$

Moreover, following the same strategy as in R-BCs, we obtain $0 \in \varrho(\mathcal{A})$. Hence, Theorem 1 holds and Theorem 2 assures the existence and uniqueness for the solution of the problem with D-BCs.

### 3.3. Strategy III: the Neumann BCs

A further strategy, which can be pursued to integrate Eqs. (1), lays upon the introduction of the following Neumann (N-) type BCs for the local heat-flux field:

$$q_{i,j}n_j = 0, \quad \forall x_i \in \partial\Omega,\ \forall t \geq 0 \tag{25}$$

Equation (25), stating that the normal derivative of the local heat flux attains a vanishing value at the walls, directly arises from the R-BCs in Eq. (15) when $C \to +\infty$, namely, when the specular phonon–wall scatterings are predominant: for this reason, Eq. (25) could be also named as *specular* BCs.

In 1D situations the above N-BCs become

$$h_{\mathsf{x}}(0,\mathsf{t}) = 0, \quad \forall \mathsf{t} \in \mathbb{R}^+ \tag{26a}$$

$$h_{\mathsf{x}}(1,\mathsf{t}) = 0, \quad \forall \mathsf{t} \in \mathbb{R}^+ \tag{26b}$$

when the dimensionless variables in Eqs. (5) are introduced. In this case, following Eqs. (12), N-BCs on $h$ impose D-BCs on $\vartheta$.

The well-posedness result can be achieved also here and deserve a brief discussion. Precisely, in this case Eq (23) still holds, whereas the domain of the operator $\mathcal{A}$ defined in Eq. (14) becomes

$$D(\mathcal{A}) = \left\{ \mathbf{U} \in \mathcal{H}; \quad h \in H^2(0,1), \vartheta \in H_0^1(0,1) : \right. \\ \left. h_{\mathsf{x}}(0,\mathsf{t}) = 0 \text{ and } h_{\mathsf{x}}(1,\mathsf{t}) = 0 \right\}$$

and its dissipativeness can be obtained by Eq. (20), respectively, by imposing boundary conditions. In fact it reads

$$\mathrm{Re}\langle \mathcal{A}\mathbf{U}, \mathbf{U}\rangle_{\mathcal{H}} = -\left[\|h\|^2 + 3\mathrm{Kn}^2 \|h_{\mathsf{x}}\|^2\right] \tag{27}$$

Moreover, in order to prove that $0 \in \varrho(\mathcal{A})$, by contradiction we suppose that $0 \notin \varrho(\mathcal{A})$. As observed in the case of the R-BCs, there exists $\mathbf{U} \neq 0$ in $D(\mathcal{A})$ satisfying equation $\mathcal{A}\mathbf{U} = 0$, from which, being $h_{\mathsf{x}} = 0$ and $\vartheta_{\mathsf{x}} = -h$, we obtain that $h$ is constant and $\vartheta$ a linear function of $\mathsf{x}$. Once more, from the null boundary conditions on $\vartheta$, we obtain that $\mathbf{U} = 0$, which is a contradiction.

Hence, existence and uniqueness result directly follows from Theorems 1 and 2

**Remark 4.** In the present theoretical approach to the problem of BCs setting-up, the coefficient $C$ is used to describe with continuity the transition from a regime of heat transfer wherein the specular phonon–wall scatterings are predominant (large values of $C$) to a regime of heat transfer wherein the diffusive phonon–wall scattering mechanism only matters (small values of $C$). The limit situation $C = 0$ characterizes a wall which completely absorbs the incoming phonons (modeled as flowing rigid particles, according with the approach used in Refs. [16,26] and our comments in Sect. 5).

## 4. Forms of heat-flux field: BCs in comparison

In this Section we explicitly furnish the forms of the two basic fields $h(\mathsf{x},\mathsf{t})$ and $\vartheta(\mathsf{x},\mathsf{t})$, once both the above strategies of BCs setting-up are pursued. We refer the readers to the "Appendix" at the end of this paper for a sketch of the solution method used to obtain Eqs. (28), (30) and (31). Therein the forms of the $2n$ constants $\lambda_n^1$ and $\lambda_n^2$ (appearing in those equations) can be found, as well as information about the $n$ numerical constants $\beta_n$.

Since in the present analysis we have primarily focused our attention on the role played by the heat flux at the boundaries, in this Section then we only discuss the qualitative behaviors of $h(\mathsf{x},\mathsf{t})$ in the system at hand.

### 4.1. Strategy I: the Robin BCs

Once the *slip-heat* BCs in Eqs. (16) are prescribed, Eqs. (8) yields the following forms of the basic fields $h$ and $\vartheta$:

$$h(\mathsf{x},\mathsf{t}) = \sum_{n=0}^{+\infty} \left( A_n e^{\lambda_n^1 \mathsf{t}} + B_n e^{\lambda_n^2 \mathsf{t}} \right) \cos(\gamma_n - \beta_n \mathsf{x}) \tag{28a}$$

$$\vartheta(\mathsf{x},\mathsf{t}) = \frac{\mathrm{Kn}^2}{3} \sum_{n=0}^{+\infty} \beta_n \left[ \frac{A_n}{\lambda_n^1} \left( 1 - e^{\lambda_n^1 \mathsf{t}} \right) + \frac{B_n}{\lambda_n^2} \left( 1 - e^{\lambda_n^2 \mathsf{t}} \right) \right] \sin(\gamma_n - \beta_n \mathsf{x}) \tag{28b}$$

wherein

$$\gamma_n = \arctan\left( \frac{1}{\beta_n C \mathrm{Kn}} \right), \quad \forall n \in \mathbb{N} \tag{29}$$

and the values of the several constants $A_n$ and $B_n$ arise from the initial conditions in Eqs. (10).

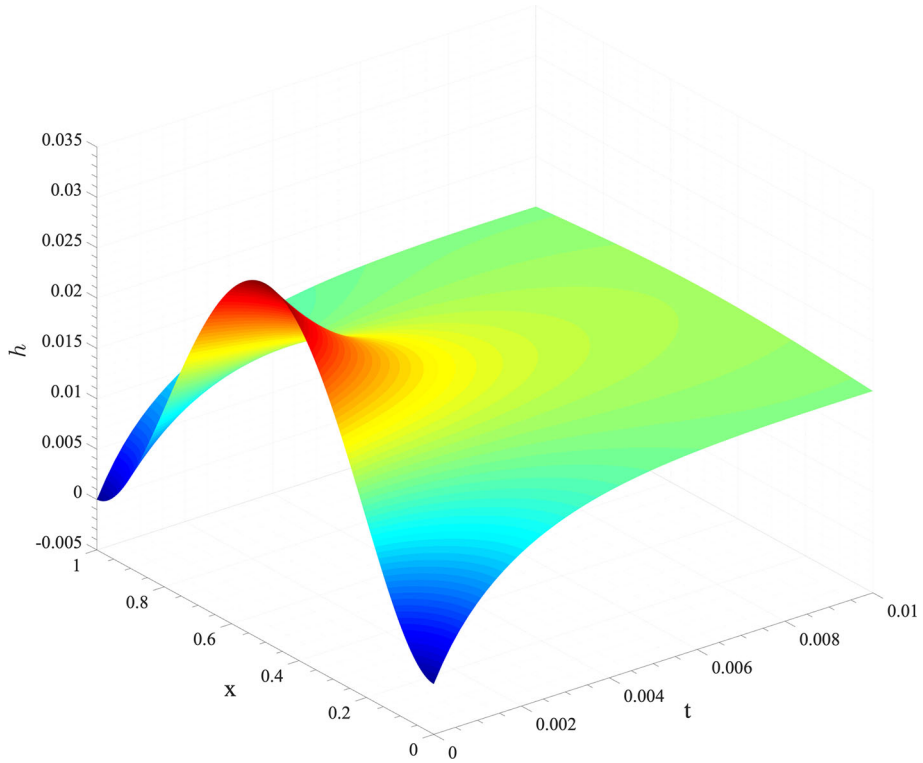


FIG. 2. R-BCs: $h$ VS $(\mathsf{x},\mathsf{t})$. Theoretical result arising from Eq. (28a). The computation has been made by assuming $C = 2.5$ and $\mathrm{Kn} = 2$

In Fig. 2 we plot the theoretical result arising from Eq. (28a). As an example, for the sake of computation, to obtain that profile we have specialized Eq. (10a) as

$$h_0(\mathsf{x}) = 1 - e^{\cos\left(\mathsf{x}^2-\mathsf{x}\right)-1}$$

### 4.2. Strategy II: the Dirichlet BCs

If the *diffusive* BCs in Eqs. (22) are prescribed, instead, Eqs. (8) yields the following forms of the basic fields $h$ and $\vartheta$:

$$h(\mathsf{x},\mathsf{t}) = \sum_{n=0}^{+\infty}\left(A_n e^{\lambda_n^1 \mathsf{t}} + B_n e^{\lambda_n^2 \mathsf{t}}\right)\cos\left(\frac{\pi}{2} - (n+1)\,\pi\mathsf{x}\right) \tag{30a}$$

$$\vartheta(\mathsf{x},\mathsf{t}) = \frac{\mathrm{Kn}^2}{3}\sum_{n=0}^{+\infty}(n+1)\,\pi\left[\frac{A_n}{\lambda_n^1}\left(1 - e^{\lambda_n^1 \mathsf{t}}\right) + \frac{B_n}{\lambda_n^2}\left(1 - e^{\lambda_n^2 \mathsf{t}}\right)\right]\sin\left(\frac{\pi}{2} - (n+1)\,\pi\mathsf{x}\right) \tag{30b}$$

with the values of the several constants $A_n$ and $B_n$ being given by the initial conditions in Eqs. (10). Note that Eqs. (30) directly arise from Eqs. (28)–(29) when $C \to 0^+$ therein.

In Fig. 3 we plot the theoretical results arising from Eq. (30a): for the sake of computation, to obtain that profile we have specialized Eq. (10a) as

$$h_0(\mathsf{x}) = 1 - e^{\cos\left(\mathsf{x}^2-\mathsf{x}\right)-1}$$

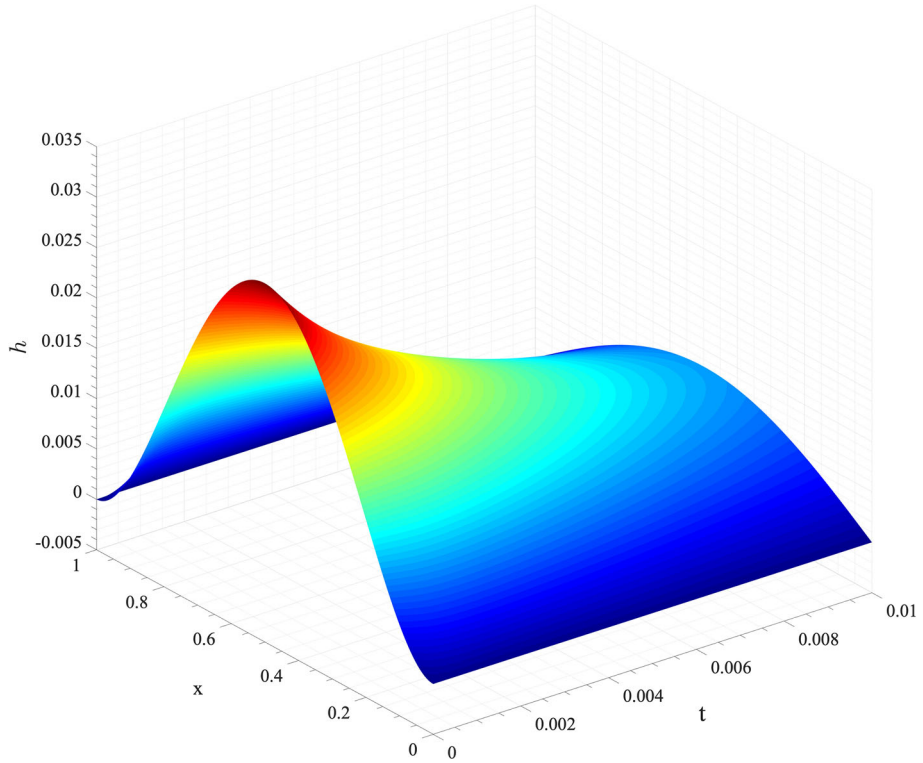


FIG. 3. D-BCs: $h$ VS $(\mathsf{x},\mathsf{t})$. Theoretical result arising from Eq. (30a). The computation has been made by assuming $\mathrm{Kn}=2$

### 4.3. Strategy III: the Neumann BCs

The *specular* BCs in Eqs. (26), instead, allow to obtain the following forms of the basic fields $h$ and $\vartheta$ from Eqs. (8):

$$h(\mathsf{x},\mathsf{t}) = \sum_{n=0}^{+\infty} \left( A_n e^{\lambda_n^1 \mathsf{t}} + B_n e^{\lambda_n^2 \mathsf{t}} \right) \cos\left((n+1)\,\pi \mathsf{x}\right) \tag{31a}$$

$$\vartheta(\mathsf{x},\mathsf{t}) = -\frac{\mathrm{Kn}^2}{3} \sum_{n=0}^{+\infty} (n+1)\,\pi \left[ \frac{A_n}{\lambda_n^1} \left( 1 - e^{\lambda_n^1 \mathsf{t}} \right) + \frac{B_n}{\lambda_n^2} \left( 1 - e^{\lambda_n^2 \mathsf{t}} \right) \right] \sin\left((n+1)\,\pi \mathsf{x}\right) \tag{31b}$$

with the values of the several constants $A_n$ and $B_n$ being given by the initial conditions in Eqs. (10). Note that Eqs. (31) directly arise from Eqs. (28)–(29) when $C \to +\infty$ therein.

In Fig. 4 we plot the theoretical result arising from Eq. (31a). As an example, for the sake of computation, to obtain that profile, we have specialized Eq. (10a) as

$$h_0(\mathsf{x}) = 1 - e^{\cos\left(\mathsf{x}^2 - \mathsf{x}\right) - 1}$$

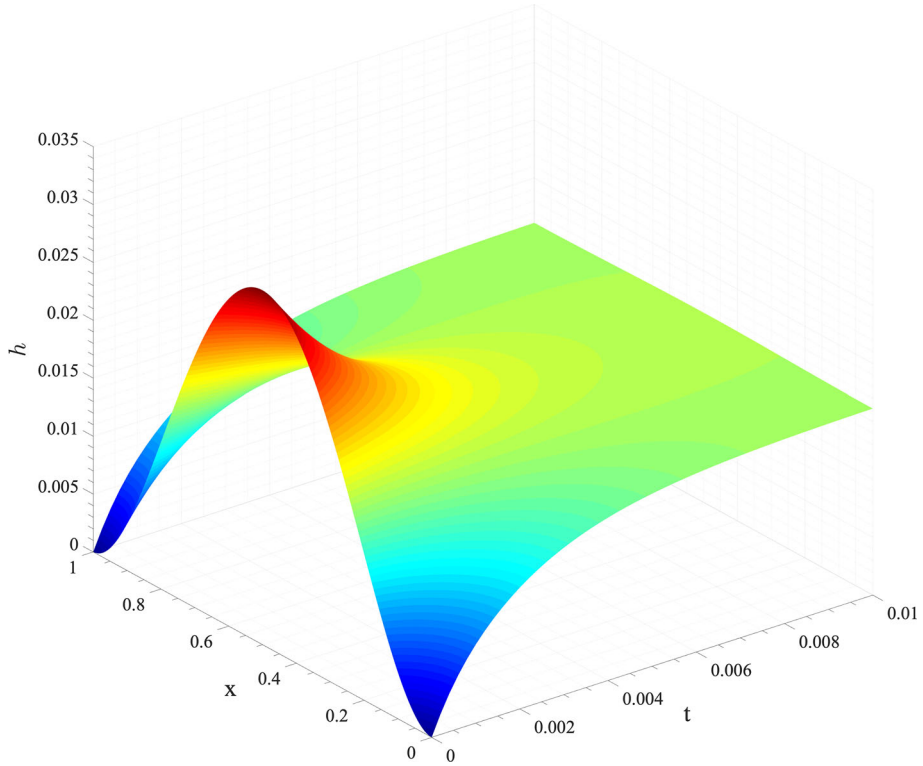


FIG. 4. N-BCs: $h$ VS $(\mathsf{x},\mathsf{t})$. Theoretical result arising from Eq. (31a). The computation has been made by assuming Kn = 2

### 4.4. BCs in comparison: role of the different mechanisms of phonon–wall scattering

Although the shapes of the unknown basic field $h(\mathsf{x},\mathsf{t})$ plotted in Figs. 2, 3 and 4 are related to the particular ID in Eqs. (10), some interesting considerations on the role played by the different BCs (i.e., the different mechanisms of phonon–wall scattering) can be however pointed out by their analysis. First of all, as it was naturally expected owing to dissipative effects, from those figures it is possible to see that (in all the situations under consideration in the present paper) the field $h(\mathsf{x},\mathsf{t})$ tends to a steady profile which is characterized by heat-flux plateau values lower than the initial ones in any point of $\Omega$. In particular, in the cases of slip-heat and specular BCs the heat-flux profile tends to the steady profile faster than in the case of diffusive BCs. Although being a very fast process in any situations, this is a tantamount to claim that in latter case the system reaches its thermodynamic equilibrium slower than in the two former cases: therefore in $\Omega$ the local equilibrium seems to be reached as more slowly as the diffusive phonon–wall scatterings are more predominant with respect to the specular phonon–wall scatterings. Incidentally, we also underline that in $\Omega$ the equilibrium is characterized by a flat profile of $h(\mathsf{x},\mathsf{t})$ both in the case of Eqs. (16), and in the case of Eqs. (26), whereas it is not uniform in the case of Eqs. (22). Similar results have been obtained in Ref. [24], for example.

From Figs. 2, 3 and 4 it is also interesting to point out that the heat-flux plateau value attained both in the case of Eqs. (16), and in the case of Eqs. (26), will be higher than the heat-flux plateau value attained in the case of Eqs. (22). This result was indeed expected owing to the non-vanishing values of the heat flux at the lateral walls predicted by the BCs in Eqs. (16) and (26): the above plateau values of the heat flux (which characterize the thermodynamic equilibrium of the systems), in fact, are clearly

related to heat flux at the boundary. Noticing that the heat-flux value at the equilibrium is substantially related to the energy which has been stored by (or transferred to) the system, the observation above could be useful for practical applications at nanoscale since one of the aspects which is currently studied is the heat removal and the consequent cooling of very small areas heated by some external source, either static (as hot spot due to a very miniaturized working device), or a fast laser pulse, for instance. Starting from this observation, a possible interesting role of the system's boundary seems to come out: $\partial\Omega$, in fact, could be modeled for own needs, instead of changing the characteristic dimensions of the system.

On the other hand, it seems also worth observing that the theoretical profiles in Figs. 2 and 4 are practically the same; although a more exhaustive analysis is required, at the present stage we suppose that this may be fundamentally due to the role played by the Knudsen number (which characterizes the particular regime of heat transfer, according to Remark 2), too: Eq. (26), in fact, can be not only viewed as the limit of Eqs. (16) for very large values of $C$, but also as the limit of Eqs. (16) for very high values of Kn (which is related to $\ell$, according with Eq. (9)).

Since the phonon mean-free path is also related to the material of the system at hand, depending on the aimed needs, the above observations point out that one should always look for the best combination between the material and the boundary's shape of the system at hand.

## 5. Conclusions

In non-metallic materials the heat-transfer phenomenon is fundamentally due to phonons. Depending on the comparison between the characteristic size $l$ of the system at hand and the phonon mean-free path $\ell$, the phonons may undergo different regimes. When $l \gg \ell$, in fact, the mechanism of phonon-bulk scattering is predominant: the heat transfer is diffusive and it can be correctly described by the usual Fourier law. Whenever $l \leq \ell$, instead, phonon–wall scatterings predominate over phonon-bulk scatterings, and the heat-transport regime may be either hydrodynamic, or ballistic. In these two cases, the Fourier law breaks down [3,9,31,32]. Among the different theories and/or approaches which have been developed to face with the breakdown of the Fourier law at nanoscale and to describe thermal transport in nanosystems, a special attention should be put on the phonon hydrodynamics [5,16,23,24,26] since it connects mesoscopic and microscopic approaches. On the other hand, an interesting question is whether phonon–wall collisions should be taken into account in prescribing the BCs for the local heat-flux value, or not, whenever the Fourier law is no longer applicable. To this end, it seems worth noticing that in nanosystems the surface scattering is expected to play an important role [16,33–38] in such a way that, for example, thermal perturbations across the transversal section of a layer are well described by an effective thermal conductivity which decreases for decreasing thickness of the layer [16,37].

Our answer to the above question is affirmative: therefore in this paper we look at a possible strategy which can be used to predict the two basic fields $T$ and $q_i$ from the heat-transfer model in Eqs. (1). In particular, by considering the thermal transport within a strip (i.e., a nanolayer wherein the thickness is much smaller than its other two characteristic sizes, see Fig. 1 for a qualitative picture of the problem at hand) we have focused our analysis in a cross section $\Omega$ of it which indeed reduces to a line, thus sketching a 1D nanosystem. Hence, the domain of our interest is the 1D interval $[0, l]$ which has been scaled to $[0, 1]$ for computational convenience by means of Eqs. (5). In this domain, we imposed that the perturbation from the local equilibrium is obtained by the application of an external heat flux perpendicular to $\Omega$ wherein we are interested to evaluate the consequent heat transfer (as sketched in Fig. 1). In doing this we underline that, on a mesoscopic level, in our approach the heat flux is only the consequence of moving heat carriers [16,24,26] which in our case are only the phonons. On the light of this observation, in any time, all the phonons inside $\Omega$ will give a *positive* contribution to the local heat flux: they certainly cross that section. The same cannot be said, instead, for the phonons that collide with the lateral walls $\partial\Omega$ which, therefore, should deserve a detailed discussion: depending on the particular phonon–wall interactions, in

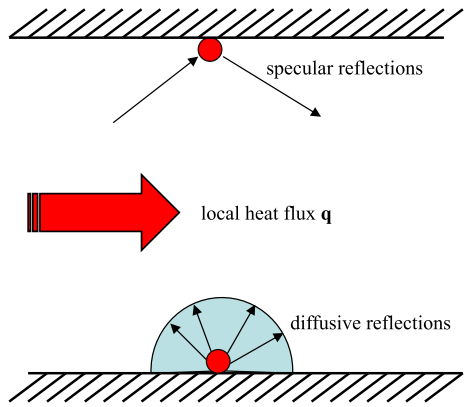


FIG. 5. Interaction of the phonons with the wall. Specular reflections yield that the phonons are reflected with an angle of reflection equal to the angle of incidence. Diffusive reflections involve the possible consequent motion of the phonons in all directions. The circle (red in figure) stands for a phonon hitting the lateral wall (color figure online)

fact, after the collision a phonon may either continues to move in the positive $z$ direction, or turn back and move in the negative $z$ direction. For this reason, in a first approach, we can classify the above interactions in two different types: specular and diffusive. In the former case, after the collision, the phonon moves in the positive direction with an angle of reflection equal to the angle of incidence; in the latter case, instead, all the directions of reflection are equiprobable after the collision. Both the above two different types of phonon–wall interactions are qualitatively sketched in Fig. 5.

Since those reflections could sensibly modify the number of the phonons crossing $\Omega$, in our approach we strategically insert them into the BCs setting-up, thus prescribing them on the heat flux. Precisely, the general possibility that both specular and diffusive interactions occur is included into the slip-heat R-BCs in Eq. (15) that finds its original physical root in the phonon-hydrodynamic approach [16,24,26] which regards the whole set of heat carriers as free particles of a gas in a box [39], the hydrodynamic-like equations of which describe the heat transport [26,40]. The occurrence in which one type of those interactions is predominant with respect to the other is instead meant as a particular case (or a limiting case, depending on the actual value of $C$) of Eq. (15) in our approach. In particular

i. when the diffusive reflections are completely predominant with respect to the specular ones Eq. (15) reduces to Eq. (21), namely, the diffusive D-BCs hold;
ii. when the specular reflections are completely predominant with respect to the diffusive ones Eq. (15) reduces to Eq. (25), namely, the specular N-BCs hold.

We note that the drastic BC in Eq. (21), holding when the number of diffusive reflections is sensibly higher than the number of specular reflections, in our approach directly arises from the observation that in principle, since all the reflection directions have the same probability of occurring, the average number of phonons going forward is null: in a certain sense, the boundary is able to stop all the incoming hitting phonons.

All these observations may explain why, in contrast with the usual approaches, we propose a novel approach to BCs, setting them on the local heat-flux field, instead of on the temperature field. It is also important to note that our approach, that is substantially related to the way as the phonon–wall interactions are included in the model, is reflected in Eq. (1b) that has indeed an important differences with respect to the original proposal of Guyer and Krumhansl [2]. In Ref. [2], the authors include the phonon–wall interactions in the relaxation time and in the consequent effective thermal conductivity appearing in the model equations. Precisely, in order to estimate $\tau$, they combine a relaxation time $\tau_{\mathrm{b}}$ (due to phonon–wall interactions) with the usual relaxation time due to the bulk resistive mechanisms

by means of the Matthiessen rule as

$$\frac{1}{\tau} = \frac{1}{\tau_{\mathrm{u}}} + \frac{1}{\tau_{\mathrm{i}}} + \frac{1}{\tau_{\mathrm{d}}} + \frac{1}{\tau_{\mathrm{b}}}$$

being $\tau_{\mathrm{u}}$ the relaxation time of umklapp phonon-phonon collisions, $\tau_{\mathrm{i}}$ the relaxation time of phonon-impurity collisions, and $\tau_{\mathrm{d}}$ the relaxation time of phonon-defect collisions. Once the combined resistive-boundary collision time is so obtained, an effective thermal conductivity $\kappa_{\mathrm{eff}}$ (depending on the size of the system through $\tau_{\mathrm{b}}$) was calculated as in Eq. (7) and then it is used in the third term of the left-hand side of Eq. (1b). In our approach, instead,

i. the phonon-boundary collisions do not display any contribution in $\tau$, but they are directly included in the BCs by means of the heat flux;
ii. we assume that $\kappa$ in Eq. (1b) is the usual bulk thermal conductivity, and not the effective one as done in Ref. [2].

At the very end we remark that, in our approach to the BCs setting-up problem, an important role is played by the (positive and non-dimensional) coefficient $C$. As aforementioned observed, in fact, Eq. (15) yields both Eq. (21) for vanishing values of $C$, and Eq. (25) for very high values of $C$. In principle, that parameter can be related to the combination of diffusive and specular phonon–wall scattering as [16,24,26]

$$C = 2\left(\frac{1+p}{1-p}\right)\xi \tag{32}$$

with $p \in (0,1)$ being the relative number of phonon–wall specular collisions as compared to the total number of specular and diffusive collisions, according with the kinetic theory of rarefied gases and electrons [22,41,42], and $\xi$ being a positive numerical constant (smaller than 1 [17]) which models the mechanical features of the lateral walls. In Ref. [37], for example, that parameter has been related both to the root-mean-square value of the roughness fluctuations, and to the average distance between roughness peaks. Hence, large values of $C$ mean that the specular phonon–wall scattering dominates over the diffusive one; conversely, small values of $C$ mean that diffusive phonon–wall collisions are predominant over specular ones. Along with this point view the BCs in Eq. (21) (which are more restrictive in comparison with the other BCs used in the present paper), besides the situation of an adiabatically isolated system, may also model the circumstance in which the phonon–wall interactions lead to a suppression of the heat flux at the boundary, thus recalling the idea of the metal-insulator Anderson transition [43,44] which can be found in amorphous systems, for example, wherein the atomic disorder is so high that extended electron states become suppressed and only localized electron states remain, which do not allow a long-range electron current. A reduction in the heat flux may in principle arises from the localization due to quantum effects: indeed, when the radius of a nanowire becomes very small, for example, in view of the Heisenberg principle, it follows that the transversal speed of the particles must become high, thus reducing the energy going along the nanowire, as a fraction of the total energy will be removed from the longitudinal dimension to feed the energy of the transversal direction. Thus, even in smooth walls, for sufficiently thin nanowires, quantum localization effects could strongly reduce the total heat flux beyond the reduction implied by classical collisions of phonons with the walls [26]. This possibility, which should deserve deeper investigation, allows us to claim that the present study about the setting-up of BCs, although encompassing a quite comprehensive overview of mechanisms of phonon–wall interactions, is however still far from its final end; a refined model of BCs, for example, should also account for the phonon backscattering, namely, the possibility that in a very narrow region close to the walls the local heat flux may also have the same direction of the temperature gradient [26,37].

## Acknowledgements

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## Appendix

For the sake of a pedagogical goal, here we furnish some details about the mathematical method used to solve Eqs. (8) when Eqs. (16), (22) and (26) are prescribed as BCs. Indeed, as a direct consequence of Eqs. (8), we firstly have

$$\vartheta_{\mathsf{tx}} + \frac{\mathrm{Kn}^2}{3} h_{\mathsf{xx}} = 0$$
$$h_{\mathsf{tt}} + h_{\mathsf{t}} + \vartheta_{\mathsf{xt}} - 3\mathrm{Kn}^2 h_{\mathsf{xxt}} = 0$$

which then yield

$$h_{\mathsf{tt}} + h_{\mathsf{t}} - \frac{\mathrm{Kn}^2}{3} h_{\mathsf{xx}} - 3\mathrm{Kn}^2 h_{\mathsf{xxt}} = 0 \tag{33}$$

The so-called *Fourier method* suggests to find the solution of Eq. (33) in the form

$$h(\mathsf{x},\mathsf{t}) = G(\mathsf{x})\, F(\mathsf{t}), \quad \forall\, (\mathsf{x},\mathsf{t}) \in [0,1] \times [0,\infty) \tag{34}$$

wherein $G$ and $F$ are two regular scalar-valued functions of the indicated arguments. Since the coupling of Eqs. (33) and (34) it turns out

$$\frac{G''}{G} = \frac{F'' + F'}{3\mathrm{Kn}^2 F' + \frac{\mathrm{Kn}^2}{3} F}\,. \tag{35}$$

From the above relation, it is easy matter to observe that the two above functions $G = G(\mathsf{x})$ and $F = F(\mathsf{t})$ have to fulfill, respectively, the following ODEs

$$G'' - \alpha G = 0 \tag{36a}$$
$$F'' + F' - \alpha \left( 3\mathrm{Kn}^2 F' + \frac{\mathrm{Kn}^2}{3} F \right) = 0 \tag{36b}$$

with $\alpha \in \mathbb{R}$, in principle.

The solutions of ODEs (36) are clearly influenced by the sign (and the value) of $\alpha$, which has to be such that the following *Sturm–Liouville* (SL) problems do not admit the only trivial solution $G(\mathsf{x}) = 0$, $\forall \mathsf{x} \in [0,1]$. Thus:

(I)

$$\begin{cases} G'' - \alpha G = 0 \\ G(0) - C\mathrm{Kn}G'(0) = 0 \\ G(1) + C\mathrm{Kn}G'(1) = 0 \end{cases} \tag{37}$$

when the R-BCs (16) have been assigned,

(II)

$$\begin{cases} G'' - \alpha G = 0 \\ G(0) = 0 \\ G(1) = 0 \end{cases} \tag{38}$$

when the D-BCs (22) hold. Note that the SL problem (38) directly arises from the SL problem (37) when $C \to 0^+$ (the diffusive phonon–wall scatterings being predominant).

(III)

$$\begin{cases} G'' - \alpha G = 0 \\ G'(0) = 0 \\ G'(1) = 0 \end{cases} \tag{39}$$

when the N-BCs (26) hold. Note that the SL problem (39) directly arises from the SL problem (37) when $C \to +\infty$ (the specular phonon–wall scatterings being predominant).

In order to have information about $\alpha$, the following result can be used.

**Theorem 3.** *Let $G : [0,1] \mapsto \mathbb{R}$ the general solution of ODE (36a). The SL problems (37)–(39) display nontrivial solutions if, and only if, $\alpha < 0$.*

*Proof.* To prove Theorem 3, it can be useful to distinguish the following cases.

**Case 1**: $\alpha = 0$

In this case Eq. (36a) yields

$$G(\mathsf{x}) = \widehat{A}\mathsf{x} + \widehat{B} \tag{40}$$

and, consequently, by direct calculations we obtain what follows.

(I) The SL problem (37) does not admit the only trivial solution if, and only if,

$$1 + 2C\mathrm{Kn} = 0$$

which is only fulfilled for the unphysical condition $2C\mathrm{Kn} = -1$ (according with the aforementioned considerations about $C$ and Kn: both of them are positive constants).

(II) The SL problem (38) always admits the only solution $G(\mathsf{x}) = 0$, $\forall \mathsf{x} \in [0,1]$.

(III) The SL problem (39) has no solutions.

**Case 2**: $\alpha > 0$

In this case Eq. (36a) yields

$$G(\mathsf{x}) = \widehat{A}e^{-\sqrt{\alpha}\mathsf{x}} + \widehat{B}e^{\sqrt{\alpha}\mathsf{x}} \tag{41}$$

Recalling what previously said about the case $\alpha = 0$, the considerations below are enough to claim that $\alpha$ cannot be a positive value, if the only trivial solution $G(\mathsf{x}) = 0$, $\forall \mathsf{x} \in [0,1]$, is not desired.

(I) The SL problem (37) does not admit the only trivial solution if, and only if,

$$\left(1 + \sqrt{\alpha}C\mathrm{Kn}\right)^2 e^{\sqrt{\alpha}} - \left(1 - \sqrt{\alpha}C\mathrm{Kn}\right)^2 e^{-\sqrt{\alpha}} = 0 \tag{42}$$

which is only fulfilled if $\alpha = 0$ therein (whatever the value of $C\mathrm{Kn}$ is).

(II) The SL problem (38) does not admit the only trivial solution if, and only if,

$$e^{\sqrt{\alpha}} - e^{-\sqrt{\alpha}} = 0$$

which is only fulfilled if $\alpha = 0$ therein. Note that the above relation directly arises from Eq. (42) when $C \to 0^+$ therein.

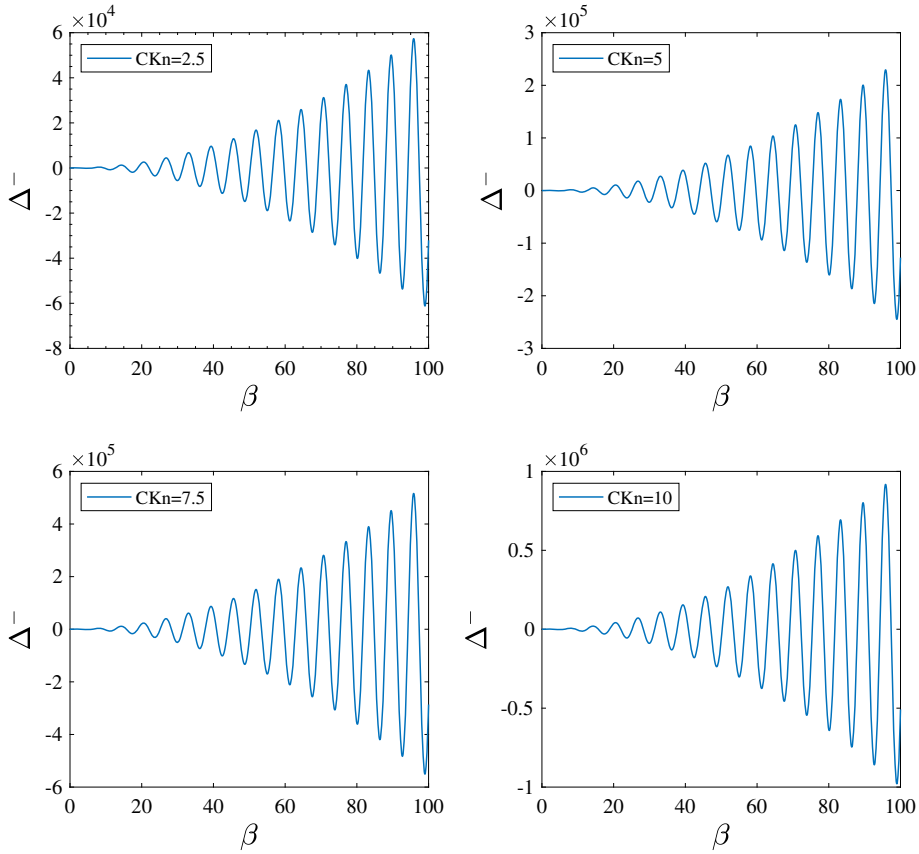


FIG. 6. $\Delta^-$ versus $\beta$ for different values of $C$Kn: results arising from Eq. (44)

(III) The SL problem (39) does not admit the only trivial solution if, and only if,

$$\alpha\left(e^{\sqrt{\alpha}}-e^{-\sqrt{\alpha}}\right)=0$$

which is only fulfilled if $\alpha = 0$ therein. Note that the above relation directly arises from Eq. (42) when $C \to +\infty$ therein.

**Case 3**: $\alpha < 0$

In this case Eq. (36a) yields

$$G(\mathsf{x}) = \widehat{A}\cos(\beta\mathsf{x}) + \widehat{B}\sin(\beta\mathsf{x}) \tag{43}$$

wherein we set $\beta := \sqrt{|\alpha|}$ just for the sake of a simple notation. Straightforward calculations point out the following results.

(I) The SL problem (37) does not admit the only trivial solution if, and only if, $\beta$ is a zero of the following function:

$$\Delta^- := \sin\beta\left[\beta^2\left(C\mathrm{Kn}\right)^2-1\right]-2\beta C\mathrm{Kn}\cos\beta \tag{44}$$

As it can be clearly seen from Fig. 6 (wherein we plot $\Delta^-$ versus $\beta$ for different values of $C$Kn), in addition to $\beta = 0$ (which is not admissible according with what previously pointed out), the $\Delta^-$ function displays $n$ (infinite) zeros.

(II) The SL problem (38) does not admit the only trivial solution if, and only if, the condition $\sin\beta = 0$ holds, namely, if $\beta = (n+1)\,\pi$, $\forall n \in \mathbb{N}$. We note that this result directly arises by checking the zeros of the $\Delta^-$ function above when $C \to 0^+$.

(III) The SL problem (39) does not admit the only trivial solution if, and only if, the condition $\beta^2 \sin\beta = 0$ holds, namely, if $\beta = (n+1)\,\pi$, $\forall n \in \mathbb{N}$. We note that this result directly arises by checking the zeros of the $\Delta^-$ function above when $C \to +\infty$.

The considerations above are enough to prove Theorem 3. □

**Remark 5.** Equation (44) cannot be indeed analytically solved. Its infinite solutions are clearly scalar-valued functions of the type $\beta_n = \beta_n(C, \mathrm{Kn})$. Since those functions do not have analytical expressions, therefore, they are only indicated by $\beta_n$ in Eqs. (28). From the aforementioned considerations, however, we may infer that

$$\lim_{C\to 0^+} \beta_n = n\pi, \qquad \forall n \in \mathbb{N}$$
$$\lim_{C\to +\infty} \beta_n = n\pi, \qquad \forall n \in \mathbb{N}$$

As a direct consequence of the results above, we have:

(I) The SL problem (37) admits $n$ (infinite) eigenvalues $\beta_n$. The corresponding eigenfunctions are

$$G_n(\mathsf{x}) = D_n^R \cos(\gamma_n - \beta_n \mathsf{x}), \quad \forall n \in \mathbb{N} \tag{45}$$

with $\gamma_n$ being given by Eq. (29), and $D_n^R$ are suitable (infinite) numerical constants. The values of $\beta_n$ also influence the solutions of ODE (36b) which, however, read

$$F_n(\mathsf{t}) = \overline{A}_n e^{\lambda_n^1 \mathsf{t}} + \overline{B}_n e^{\lambda_n^2 \mathsf{t}}, \quad \forall n \in \mathbb{N} \tag{46}$$

wherein we have

$$\lambda_n^{1,2} = -\left(\frac{1+3\beta_n^2\mathrm{Kn}^2}{2}\right)\left[1 \mp \sqrt{1-\frac{4}{3}\left(\frac{\beta_n \mathrm{Kn}}{1+3\beta_n^2\mathrm{Kn}^2}\right)^2}\right] \tag{47}$$

Incidentally we note that $\lambda_n^{1,2} < 0$, $\forall n \in \mathbb{N}$.
The coupling of Eqs. (45) and (46) allows us to obtain Eq. (28a) which, in turn, gives Eq. (28b) from Eq. (11).

(II) The SL problem (38) admits the $n$ (infinite) eigenvalues $\beta_n := (n+1)\,\pi$, $\forall n \in \mathbb{N}$. The corresponding eigenfunctions are

$$G_n(\mathsf{x}) = D_n^D \cos\left(\frac{\pi}{2} - (n+1)\,\pi\mathsf{x}\right), \quad \forall n \in \mathbb{N} \tag{48}$$

with $D_n^D$ being suitable (infinite) numerical constants. When those eigenvalues are inserted into ODE (36b), straightforward calculations allow us to obtain again Eq. (46) with

$$\lambda_n^{1,2} = -\left[\frac{1+3\pi^2(n+1)^2\mathrm{Kn}^2}{2}\right]\left\{1 \mp \sqrt{1-\frac{4}{3}\left[\frac{(n+1)\,\pi\mathrm{Kn}}{1+3\pi^2(n+1)^2\mathrm{Kn}^2}\right]^2}\right\} \tag{49}$$

in this case. We also note that Eqs. (48) and (49) directly arise from Eqs. (45) and (47), respectively, when $C \to 0^+$. It is also worth noticing that $\lambda_n^{1,2} < 0$, $\forall n \in \mathbb{N}$ again.
The coupling of Eqs. (46) and (48) allows us to obtain Eq. (30a) which, in turn, gives Eq. (30b) from Eq. (11).

(III) The SL problem (39) admits the $n$ (infinite) eigenvalues $\beta_n := (n+1)\,\pi$, $\forall n \in \mathbb{N}$, too. The corresponding eigenfunctions, instead, are

$$G_n(\mathsf{x}) = D_n^N \cos((n+1)\,\pi\mathsf{x}), \quad \forall n \in \mathbb{N} \tag{50}$$

with $D_n^N$ suitable (infinite) numerical constants. When those eigenvalues are inserted into ODE (36b), straightforward calculations allow us to obtain again Eq. (46) with $\lambda_n^{1,2}$ still given by Eq. (49). We also note that Eqs. (50) and (49) directly arise from Eqs. (45) and (47), respectively, when $C \to +\infty$. The coupling of Eqs. (46) and (50) allows us to obtain Eq. (31a) which, in turn, gives Eq. (31b) from Eq. (11).

Equations (28), (30) and (31) contain the $2n$ numerical constants $A_n$ and $B_n$. In order to determine all of them we need to prescribe two independent sets of $n$ linear algebraic equations.

The first set arises from the initial condition on the heat flux, i.e., Eq. (10a), and reads:

(i) $h_0(\mathsf{x}) = \sum_{k=0}^{n} (A_k + B_k) \cos(\gamma_k - \beta_k \mathsf{x}), \quad \forall n \in \mathbb{N}$
in the case of R-BCs.

(ii) $h_0(\mathsf{x}) = \sum_{k=0}^{n} (A_k + B_k) \sin((n+1)\pi \mathsf{x}), \quad \forall n \in \mathbb{N}$
in the case of D-BCs. Note that this set of linear algebraic equations directly follows from the set i) above when $C \to 0^+$ therein.

(iii) $h_0(\mathsf{x}) = \sum_{k=0}^{n} (A_k + B_k) \cos((n+1)\pi \mathsf{x}), \quad \forall n \in \mathbb{N}$
in the case of N-BCs. Note that this set of linear algebraic equations directly follows from the set i) above when $C \to +\infty$ therein.

The second set of $n$ linear algebraic equations cannot be obtained by the initial condition on the temperature: Eqs. (28b), (30b) and (31b), in fact, trivially give $\vartheta(\mathsf{x}, \mathsf{t}) = 0$ at the initial time $\mathsf{t} := 0$, and no conditions on the numerical constants $A_n$ and $B_n$ can be therefore obtained. On the other hand, by requiring that Eqs. (28) (in the case of the R-BCs), (30) (in the case of the D-BCs), and (31) (in the case of the N-BCs) always (i.e., $\forall (\mathsf{x}, \mathsf{t}) \in [0,1] \times (0, +\infty)$) fulfill Eq. (8), straightforward calculations allow us to obtain the following second set of $n$ linear algebraic equations

(i) in the case of R-BCs

$$0 = \frac{\mathrm{Kn}^2}{3} \sum_{k=0}^{n} \beta_k^2 \left( \frac{A_k}{\lambda_k^1} + \frac{B_k}{\lambda_k^2} \right) \cos(\gamma_k - \beta_k \mathsf{x}), \quad \forall n \in \mathbb{N} \tag{51}$$

with $\lambda_n^1$ and $\lambda_n^2$ being given by Eq. (47).

(ii) in the case of D-BCs

$$0 = \frac{\mathrm{Kn}^2}{3} \sum_{k=0}^{n} \pi^2 (k+1)^2 \left( \frac{A_k}{\lambda_k^1} + \frac{B_k}{\lambda_k^2} \right) \sin((k+1)\pi \mathsf{x}), \quad \forall n \in \mathbb{N} \tag{52}$$

with $\lambda_n^1$ and $\lambda_n^2$ being given by Eq. (49).
Note that Eqs. (52), remembering Eqs. (29), arises from Eq. (51) when $C \to 0^+$ therein.

(iii) in the case of N-BCs

$$0 = \frac{\mathrm{Kn}^2}{3} \sum_{k=0}^{n} \pi^2 (k+1)^2 \left( \frac{A_k}{\lambda_k^1} + \frac{B_k}{\lambda_k^2} \right) \cos((k+1)\pi \mathsf{x}), \quad \forall n \in \mathbb{N} \tag{53}$$

with $\lambda_n^1$ and $\lambda_n^2$ being still given by Eq. (49).
Note that also in this case Eq (53), remembering Eq (29), arises from Eq. (51) when $C \to +\infty$ therein.

**Remark 6.** Both from the coupling of Eqs. (28b) and (51) (in the case of *slip-heat* BCs), and from the coupling of Eqs. (30b) and (52) (in the case of *diffusive* BCs), as well as from the coupling of Eqs. (31b) and (53) (in the case of *specular* BCs), we may turn out that $\vartheta(\mathsf{x}, \mathsf{t}) \to 0$ when $\mathsf{t} \to +\infty$: from the practical point of view, me may therefore claim that the system at hand turns back to an equilibrium state when $\mathsf{t} \to +\infty$. This is a condition which is physically expected, if one also observes that $h(0, \mathsf{t}) \to 0$ when $\mathsf{t} \to +\infty$ in all the BC strategies analyzed.

## References


[1] Guyer, R.A., Krumhansl, J.A.: Solution of the linearized phonon Boltzmann equation. Phys. Rev. **148**, 766–778 (1966)
[2] Guyer, R.A., Krumhansl, J.A.: Thermal conductivity, second sound and phonon hydrodynamic phenomena in nonmetallic crystals. Phys. Rev. **148**, 778–788 (1966)
[3] Grmela, M., Lebon, G., Dauby, P.C., Bousmina, M.: Ballistic-diffusive heat conduction at nanoscale: GENERIC approach. Phys. Lett. A **339**, 237–245 (2005)
[4] Lebon, G., Jou, D., Casas-Vázquez, J.: Understanding Non-equilibrium Thermodynamics. Springer, Berlin (2008)
[5] Jou, D., Casas-Vázquez, J., Lebon, G.: Extended Irreversible Thermodynamics, 4th edn. Springer, Berlin (2010)
[6] 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)
[7] Dong, Y., Cao, B.-Y., Guo, Z.-Y.: Temperature in nonequilibrium states and non-Fourier heat conduction. Phys. Rev. E **87**, 032150 (2013)
[8] Serdyukov, S.I.: Higher order heat and mass transfer equations and their justification in extended irreversible thermodynamics. Theor. Found. Chem. Eng. **47**, 89–103 (2013)
[9] Tzou, D.Y.: Macro- to Microscale Heat Transfer: The Lagging Behaviour, 2nd edn. Wiley, London (2014)
[10] 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)
[11] Ruggeri, T., Sugiyama, M.: Classical and Relativistic Rational Extended Thermodynamics of Gases. Springer, Cham (2021)
[12] Casas-Vázquez, J., Jou, D.: Temperature in nonequilibrium states: a review of open problems and current proposals. Rep. Prog. Phys. **66**, 1937–2023 (2003)
[13] Puglisi, A., Sarracino, A., Vulpiani, A.: Temperature in and out of equilibrium: a review of concepts, tools and attempts. Phys. Rep. **709–710**, 1–60 (2017)
[14] Struchtrup, H., Weiss, W.: Maximum of the local entropy production becomes minimal in stationary processes. Phys. Rev. Lett. **80**, 5048 (1998)
[15] Struchtrup, H., Torrilhon, M.: $h$ theorem, regularization, and boundary conditions for linearized 13 moment equations. Phys. Rev. Lett. **99**, 014502 (2007)
[16] Alvarez, F.X., Jou, D., Sellitto, A.: Phonon hydrodynamics and phonon-boundary scattering in nanosystems. J. Appl. Phys. **105**, 014317 (2009)
[17] Xu, M.: Slip boundary condition of heat flux in Knudsen layers. Proc. R. Soc. A **470**, 20130578 (2014)
[18] Hua, Y.-C., Cao, B.: Slip boundary conditions in ballistic–diffusive heat transport in nanostructures. Nanoscale Microscale Thermophys. Eng. **21**(3), 159–176 (2017)
[19] 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)
[20] 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)
[21] Ferkl, P., Pokorný, R., Bobák, M., Kosek, J.: Heat transfer in one-dimensional micro- and nano-cellular foams. Chem. Eng. Sci. **97**, 50–58 (2013)
[22] Ziman, J.M.: Electrons and Phonons. Oxford University Press, Oxford (2001)
[23] Lee, S., Broido, D., Esfarjani, K., Chen, G.: Hydrodynamic phonon transport in suspended graphene. Nat. Commun. **6**, 6290 (2015)
[24] Sellitto, A., Carlomagno, I., Jou, D.: Two-dimensional phonon hydrodynamics in narrow strips. Proc. R. Soc. A **471**, 20150376 (2015)
[25] 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)
[26] Sellitto, A., Cimmelli, V.A., Jou, D.: Mesoscopic description of boundary effects and effective thermal conductivity in nanosystems: phonon hydrodynamics. In: Chapter 3 in Mesoscopic Theories of Heat Transport in Nanosystems. SEMA-SIMAI Springer Series, pp. 53–89. Springer (2016)
[27] Kennard, E.H.: Kinetic Theory of Gases. McGraw-Hill, New York (1938)
[28] Cercignani, C.: Slow Rarefied Flows: Theory and Application to Micro-Electro-Mechanical Systems. Birkhäuser, Basel (2006)
[29] Wu, L.: A slip model for rarefied gas flows at arbitrary Knudsen number. Appl. Phys. Lett. **93**, 253103 (2008)
[30] Pazy, A.: Semigroups of linear operators and applications to partial differential equations. In: Applied Mathematical Sciences, vol. 44. Springer, New York (1983)
[31] Chen, G.: Ballistic–diffusion equations for transient heat conduction from nano to macroscales. J. Heat Transf. Trans. ASME **124**, 320–328 (2001)

[32] Zhang, Z.M.: Nano/Microscale Heat Transfer. McGraw-Hill, New York (2007)
[33] Tešanović, Z., Jarić, M.V., Maekawa, S.: Quantum transport and surface scattering. Phys. Rev. Lett. **57**, 2760–2763 (1986)
[34] Balandin, A., Wang, K.L.: Effect of phonon confinement on the thermoelectric figure of merit of quantum wells. J. Appl. Phys. **84**, 6149 (1998)
[35] Balandin, A., Wang, K.L.: Significant decrease of the lattice thermal conductivity due to phonon confinement in a free-standing semiconductor quantum well. Phys. Rev. B **58**, 1544–1549 (1998)
[36] Bergmann, G.: Conductance of a perfect thin film with diffuse surface scattering. Phys. Rev. Lett. **94**, 106801 (2005)
[37] Sellitto, A., Alvarez, F.X., Jou, D.: Temperature dependence of boundary conditions in phonon hydrodynamics of smooth and rough nanowires. J. Appl. Phys. **107**, 114312 (2010)
[38] Márkus, F., Gambár, K.: Heat propagation dynamics in thin silicon layers. Int. J. Heat Mass Transf. **56**, 495–500 (2013)
[39] Chen, G.: Nanoscale Energy Transport and Conversion: A Parallel Treatment of Electrons, Molecules, Phonons, and Photons. Oxford University Press, Oxford (2005)
[40] Bausch, W.: Thermal conductivity and Poiseuille flow of phonons in dielectric films and plates. Phys. Status Solidi B **52**, 253–262 (1972)
[41] Gombosi, T.I.: Gaskinetic Theory. Cambridge University Press, Cambridge (1994)
[42] Struchtrup, H.: Macroscopic Transport Equations for Rarefied Gas Flows: Approximation Methods in Kinetic Theory: Interaction of Mechanics and Mathematics. Springer, Heidelberg (2005)
[43] Dobrosavljević, V., Kotliar, G.: Mean field theory of the Mott–Anderson transition. Phys. Rev. Lett. **78**, 3943–3946 (1997)
[44] García-García, A.M.: Classical intermittency and quantum Anderson transition. Phys. Rev. E **69**, 066216 (2004)

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