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Effective phonon mean-free path and slip heat flow in rarefied phonon hydrodynamics

I. Carlomagno [a,*], A. Sellitto [a], D. Jou [b,c]

[a] Department of Mathematics, Computer Science and Economics, University of Basilicata, Campus Macchia Romana, 85100 Potenza, Italy
[b] Departament de Física, Universitat Autònoma de Barcelona, 08193 Bellaterra, Catalonia, Spain
[c] Institut d'Estudis Catalans, Carme 47, Barcelona 08001, Catalonia, Spain

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ABSTRACT

Non-local effects in generalized heat-transport equations provide a mesoscopic approach to phonon hydrodynamics. In contrast to usual phonon hydrodynamics with non-slip heat flow, we consider, in analogy to rarefied gas dynamics, a slip heat flow along the walls. This way the effective thermal conductivity behaves as Kn^{-1} instead of as Kn^{-2}, which is the behavior in usual phonon hydrodynamics, Kn being the Knudsen number, i.e., the ratio between the mean-free path of the heat carriers and a characteristic size of the system. Here we revisit previous formulations to provide a more explicit and clearer interpretation of the differences between the effective mean-free path in the non-local term of the generalized transport equation for **q**, and that in the thermal conductivity.

1. Introduction

Non-local effects are especially relevant in heat transport in nanosystems where the characteristic size of the system becomes comparable to (or smaller than) the mean-free path of the heat carriers, especially phonons. In this case, not only resistive (specular and diffusive) phonon collisions against the walls arise, but also collective phonon effects related to normal (momentum-conserving) phonon–phonon collisions, redistributing among phonons the total conserved momentum, as it was pointed out in detail by Guyer and Krumhansl in Refs. [1,2]. The role of these collective effects on heat transport and thermal conductivity, in contrast to the individual phonon effects of resistive collisions, has been recently developed in a kinetic-collective model of phonon heat transfer [3,4], pointing out the relevance of collective (hydrodynamics-like) regime. The special relevance of collective-hydrodynamic regime in two-dimensional systems, as for instance graphene, has been also recently emphasized [5,6]. These recent microscopic developments may give a renewed interest to previous mesoscopic phenomenological descriptions of phonon hydrodynamics [7–12].

Mesoscopic approaches to non-local heat transport and phonon hydrodynamics have been a stimulus for non-equilibrium thermodynamics beyond classical local-equilibrium regime [13–21]. A relevant problem in this frontier refers to boundary conditions for the heat flux [7,8,22,23].

Guyer and Krumhansl [1,2] considered non-slip (i.e., vanishing) conditions for the heat flux in the hydrodynamic regime. However, this may lead to a too strong reduction of the associated thermal conductivity in this regime in terms of the characteristic size of the system. In order to improve the agreement with experimental observations and with theoretical analysis of kinetic theory of rarefied gases, it has been proposed to consider a slip (i.e., non-vanishing) heat flow along the walls [7,8,10,22–25].

The phonon mean-free path and its relative value in comparison with the characteristic size of the system also becomes a relevant parameter. However, the phonon mean-free path depends on the phonon frequency and on the frequency dependence of the several collision rates, and this influences the size dependence of several aspects of heat transport [26–28]. Furthermore, the mean-free path appears in different ways in the thermal conductivity, in the non-local terms in generalized heat-transport equations, and in the slip condition along the walls.

Here, we discuss the value of the effective phonon mean-free path appearing in the generalized heat-transport equation of some mesoscopic versions of phonon hydrodynamics [7,8,12,29] as compared to the effective mean-free path derived from the thermal conductivity. We also comment on its role in the boundary conditions referring to a slip heat flow along the walls.

* Corresponding author.
E-mail addresses: isabellacarlomagno85@gmail.com (I. Carlomagno), ant.sellitto@gmail.com (A. Sellitto), david.jou@uab.cat (D. Jou).

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The paper runs in the following way. In Section 2 we present the basic equations and carry out the explicit discussion in smooth-wall nanowires. In Section 3 we generalize the discussion to rough-wall nanowires. Section 4 presents some microscopic viewpoints and a final discussion.

2. Rarefied phonon hydrodynamics: a mesoscopic approach

In the analysis of heat transport in nanosystems, memory effects (in the form of relaxational terms), as well as non-local and non-linear effects have to be taken into account [14,15,19,29]. This requires that heat-transport equations have to be more general than the classical Fourier law. In Refs. [7–10,12] it was proposed a generalized non-local heat-transport equation of the form

$$\tau_R \dot{\mathbf{q}} + \mathbf{q} = -\lambda \nabla T + a^2(T)\,\ell^2 \left(\nabla^2 \mathbf{q} + 2\nabla\nabla\cdot\mathbf{q}\right), \tag{1}$$

where $\mathbf{q}$ is the local heat flux, τ_R is the average collision time of resistive phonon collisions, related to the collision times of umklapp phonon–phonon collisions τ_u, phonon–impurity collisions τ_i, and phonon–defect collisions τ_d as

$$\tau_R^{-1} = \tau_u^{-1} + \tau_i^{-1} + \tau_d^{-1},$$

according to Matthiessen rule, λ is the bulk thermal conductivity, and ℓ is the phonon mean-free path. Moreover, in those papers the dimensionless function $a(T)$ (which will be analyzed in this paper) was taken equal to 1. It is also worth noticing that in Refs. [7–10, 12], in considering Eq. (1) it is assumed that $\ell = \mathrm{v}\tau_R$ and means the phonon mean-free path appearing in the usual simple expression for the bulk thermal conductivity

$$\lambda = \frac{1}{3} c_v \mathrm{v} \ell, \tag{2}$$

with c_v being specific heat per unit volume, and v phonon speed in the Debye approximation.

In Refs. [7,8] the authors assumed that the local heat flux $\mathbf{q}$ just arises from the sum of two different contributions: the bulk contribution $\mathbf{q}_b$ and the wall contribution $\mathbf{q}_w$. The former contribution arises from the solution of Eq. (1) for non-slip conditions along the walls, and the latter contribution, instead, is given by the following constitutive equation

$$\mathbf{q}_w = C a(T)\,\ell \left(\frac{\partial \mathbf{q}_b}{\partial r}\right)_{r=R}, \tag{3}$$

where C stands for a dimensionless coefficient (accounting for specular and diffusive reflections), and ℓ was assumed to be the same appearing in Eqs. (1) and (2). Furthermore, in Eq. (3) r means the distance from the longitudinal axis of the nanostructure at hand, and R is its characteristic size. Note that Eq. (3) is analogous to the slip condition used for the gas velocity in rarefied gas dynamics [30–32].

In this paper, we no longer assume $a(T) \equiv 1$, and investigate the influence of $a(T)\,\ell$ in describing the non-local effects both in the second term of the right-hand side of Eq. (1), and in the slip condition (3).

Indeed, in steady-state situations, from the local balance of the internal energy u per unit volume (in the absence of heat source), i.e.,

$$\dot{u} = -\nabla\cdot\mathbf{q},$$

it follows that the local heat flux is a solenoidal vector, that is, $\nabla\cdot\mathbf{q} = 0$. Owing this, whenever the heat flux can be neglected with respect to its spatial derivatives [7,8], Eq. (1) simply becomes

$$a^2\ell^2\nabla^2\mathbf{q} = \lambda\nabla T,$$

Table 1
Bulk thermal conductivity λ (W/mK) and phonon mean-free path ℓ (nm) for silicon at different values of temperature (K).

	$T=150$	$T=100$	$T=80$	$T=60$	$T=50$	$T=40$	$T=30$
λ	409	884	1340	2110	2680	3530	4810
ℓ	181	557	1432	3837	6681	11 517	16 354

Table 2
Experimental values of the effective thermal conductivity (W/mK) in silicon nanowires with different radii R (nm) and at several values of temperature T (K) in the absence of backscattering [33–35].

R	λ_{eff}						
	$T=150$	$T=100$	$T=80$	$T=60$	$T=50$	$T=40$	$T=30$
115	46	45	40	27	19	13	5
56	28	23	21	16	11	7	3
37	17	14	11	8	6	4	1.7

whose solution, combined with Eq. (3), turns out that in cylindrical nanowire the local heat flux in any transversal section is

$$q(r) = \frac{\lambda}{4a^2\ell^2}\left(R^2 - r^2 + 2Ca\ell R\right)\frac{\Delta T}{L}. \tag{4}$$

Then, if one defines the effective thermal conductivity as

$$\lambda_{\mathrm{eff}} = \left(\frac{Q_{\mathrm{tot}}}{\pi R^2}\right)\frac{L}{\Delta T}, \tag{5}$$

with $Q_{\mathrm{tot}} = \int_0^R q(r)\,2\pi r dr$ being the total heat flux along the nanowire, the coupling of Eqs. (4) and (5) leads to [7,8]

$$\lambda_{\mathrm{eff}} = \frac{\lambda}{8a^2\,\mathrm{Kn}^2}\left(1 + 4aC\,\mathrm{Kn}\right), \tag{6}$$

wherein $\mathrm{Kn} \equiv \ell/R$ is the Knudsen number, R being the radius of the transversal section of the nanowire. In the limit of small values of the ratio R/ℓ (that is, for high Knudsen numbers), Eq. (6) reduces to

$$\lambda_{\mathrm{eff}} = \frac{\lambda C}{2a\,\mathrm{Kn}}. \tag{7}$$

This linear behavior of the effective thermal conductivity in terms of Kn^{-1} is in contrast with the quadratic behavior Kn^{-2} obtained from Eq. (6) for $C = 0$, i.e., in the absence of slip heat flow, which differs from experimental behavior.

Equations (6) and (7) describe a strong reduction of the thermal conductivity in nanowires as compared to bulk thermal conductivity. In particular, the values of the bulk thermal conductivity for Si for several temperatures are given in Table 1, together with the respective value of the mean-free path as obtained from Eq. (2). In Table 2, the effective thermal conductivity for Si nanowires of several radii are given for the same temperatures as in Table 1 according to the experimental data in Refs. [33–35] in the absence of backscattering. Comparison of Tables 1 and 2 shows indeed the mentioned strong reduction.

In Ref. [8], wherein the coefficient $a(T)$ in Eq. (1) was taken equal to 1, the values of the parameter C as a function of temperature were searched to fit the data of Table 2, by using as input the data of Table 1 for $\lambda(T)$ and $\ell(T)$, and the following result was derived

$$C(T) = C_3 T^3 + C_2 T^2 + C_1 T + C_0, \tag{8}$$

with $C_0 = -1.5$, $C_1 = 9.4\times10^{-2}\,\mathrm{K}^{-1}$, $C_2 = -1.1\times10^{-3}\,\mathrm{K}^{-2}$, $C_3 = 4.0\times10^{-6}\,\mathrm{K}^{-3}$.

Though $a(T)$ in Ref. [8] could have been considered as a further fitting parameter, it was taken equal to 1 in order to keep the maximum simplicity in the phenomenological description.