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Nonequilibrium temperatures and second-sound propagation along nanowires and thin layers

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ABSTRACT

It is shown that the dispersion relation of heat waves along nanowires or thin layers could allow to compare two different definitions of nonequilibrium temperature, since thermal waves are predicted to propagate with different phase speed depending on the definition of nonequilibrium temperature being used. The difference is small, but it could be in principle measurable in nanosystems, as for instance nanowires and thin layers, in a given frequency range. Such an experiment could provide a deeper view on the problem of the definition of temperature in nonequilibrium situations.

1. Introduction

The meaning of temperature in nonequilibrium situations is a fundamental open problem in nonequilibrium thermodynamics and statistical physics [1–6]. This problem becomes especially acute in nanosystems experiencing fast processes [7–9], because of the relatively small number of particles involved and the influence of fast variations. The latter have a practical motivation because of the high frequencies at which are expected to work the miniaturized devices in computers, for instance. In such systems, the fundamental problem of the meaning of temperature may have practical relevance in the interpretation of the experimental results and, on the other side, it may find new experimental possibilities allowing to illustrate and measure the difference between the classical definition of nonequilibrium temperature, based on the local-equilibrium hypothesis [1,2,10], and a new definition of a dynamical nonequilibrium temperature regarded as an internal variable [11]. The aim of this Letter is precisely to point out a situation in which such a difference could be examined by means of the dispersion relation of heat waves along nanowires and thin layers, where the effects related to heat exchange between the system and the medium become especially relevant.

Nowadays one-dimensional devices, such as nanowires and nanotubes, have considerably attracted the attention in virtue of their potential application in electronic and energy conversion devices. Their behavior is strongly influenced by nonlocal and nonlinear effects [12–17], due to the fact that even a small difference of temperature or electrical potential, over a small-scale length may generate very high gradients [18–21]. The analysis of high-frequency thermal waves and heat pulses in these systems requires going beyond the classical Fourier law, which is restricted to rel-

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atively low frequencies, but predicts an infinite speed for heat pulses and high-frequency waves, a result which is in contradiction with the observations.

The so-called Maxwell–Cattaneo (or Maxwell–Cattaneo–Vernotte) equation [22], is the simplest transport equation leading to a finite speed propagation of thermal waves. It reads [7–9,11, 22–24]

$$\tau\dot{\mathbf{q}}+\mathbf{q}=-\lambda\nabla\theta, \tag{1}$$

where $\mathbf{q}$ is the heat flux, τ a suitable relaxation time, λ the effective heat conductivity, and θ the nonequilibrium temperature defined through the differentiation of a suitable nonequilibrium entropy, as the one used in Extended Irreversible Thermodynamics [7,23] for instance. This will be discussed in more details in Section 3. Moreover, in Eq. (1) the superposed dot means the material time derivative which for a rigid body at rest, as the system at hand is, reduces to the usual partial time derivative. It is worth noticing that the equation above is not the most general one to describe heat conduction in miniaturized systems. For instance, Chen [15] has suggested to regard the transport of heat in nanosize systems as a combination of the heat conduction described by a kinetic equation (ballistic transport) superposed to the heat conduction governed by the Cattaneo equation. The state variables are thus the fields of the energy density and the heat flux, describing the overall Cattaneo heat conduction, and the one-phonon distribution function describing the superposed on it ballistic component. The thermodynamic compatibility of such an approach has been investigated by Grmela et al. [25]. As the result, both the Cattaneo and the kinetic equations are modified by the appearance of new terms in which their coupling is expressed. Here we limit ourselves to those nonequilibrium situations which are well described by Eq. (1) only. Note that in nanowires and thin layers, namely, in systems where the radius or the width is of the order of the mean-free path, both τ and λ are size dependent, and they show a strong reduction as compared with bulk values [7,8,14–17]. However, the ratio λ/τ is expected to have only slight changes, except in very thin systems where quantum confinement effects may become relevant.

Here we will incorporate the thermal exchange across the lateral walls of the system and we will explore how this exchange may allow to discriminate the description of heat transport through Eq. (1), or through a different dynamical nonequilibrium temperature.

2. Heat conduction and nonequilibrium temperatures

The evolution equation for θ in a cylinder of radius r, or equivalently in a thin layer of thickness r, if they are not laterally isolated, is

$$c\dot{\theta}=-\nabla\cdot\mathbf{q}-\frac{2\sigma}{r}(\theta-\theta_{\mathrm{env}}), \tag{2}$$

with c as the specific heat per unit volume, and the second term in the right-hand side representing the heat flux exchanged with the surrounding environment across the lateral walls of the system. It is in accordance with the Newton cooling law, being σ a suitable heat exchange coefficient, and θ_{env} the temperature of the environment, which will be assumed to be constant and homogeneous. Furthermore, in Eq. (2) $\mathbf{q}$ stands for the longitudinal heat flux along the length of the cylinder, or along the plane of the thin layer. It is worth observing that for systems of macroscopic dimensions, a term like the last one on the right-hand side of Eq. (2) could be incorporated in the description of heat transport as a boundary condition in situations far from equilibrium. Here we apply a different point of view, according to which, due to the small dimensions of the system, not only the points of the lateral mantle but any point undergoes heat exchanges with the environment, whose rate depends on the difference of temperature, as expressed by the right-hand side of Eq. (2). In fact, Eq. (2) assumes Newton law stating that the heat flux across the lateral surface is $\mathbf{q}_{\mathrm{w}}=\sigma(\theta-\theta_{\mathrm{env}})$. Since we are assuming in Eq. (1) that the longitudinal heat flux $\mathbf{q}$ is not given by Fourier law but by the Maxwell–Cattaneo one, incorporating relaxation effects, one could ask why we have not generalized the Newton law in a similar way, namely, assuming that $\tau_{\mathrm{w}}\dot{\mathbf{q}}_{\mathrm{w}}+\mathbf{q}_{\mathrm{w}}=\sigma(\theta-\theta_{\mathrm{env}})$. The reason to neglect τ_{w} in comparison with τ (characterizing the longitudinal heat flux) is that the collision rate of phonons with the lateral surface will be much higher than the collision rate between phonons themselves. Indeed, if l is the mean-free path of heat carriers, r the radius of the cylinder and $\bar{c}$ the average phonon speed, we will have $\tau_{\mathrm{w}}=r/\bar{c}$ and $\tau=l/\bar{c}$, respectively. Since in nanotubes r is smaller, or much smaller, than the phonon mean-free path, it follows that τ_{w} may indeed be neglected in our approach. In contrast, for r longer than the mean-free path, τ_{w} should be taken into account.

A second comment refers to the validity of a single relaxation time τ in Eq. (1); in general, since there are several collision processes (elastic phonon–phonon collisions, resistive or Umklapp phonon–phonon collisions, phonon–impurity collisions, etc.) one should take all these times into account. Here we assume that the relaxation time τ used in Eq. (1) is given by the Matthiesen rule [8,26], according to which the reciprocal of the effective collision time is the sum of the reciprocal of the several collision times.

Combining Eqs. (1) and (2), if all material functions τ, c and σ are supposed to be constant, one obtains

$$\ddot{\theta}+\left(\frac{1}{\tau}+\frac{1}{\tau_r}\right)\dot{\theta}=U_0^2\nabla^2\theta-\left(\frac{\theta-\theta_{\mathrm{env}}}{\tau\tau_r}\right), \tag{3}$$

with

$$\tau_r=\frac{rc}{2\sigma}, \tag{4}$$

as the relaxation time due to the lateral dispersion of heat, and

$$U_0=\sqrt{\frac{\lambda}{c\tau}}, \tag{5}$$

as the speed of a thermal wave traveling through an equilibrium state. Note that τ_r expresses the time-lag due to the heat exchange of the lateral mantle only, but it is not related to phonons collisions processes, which have been all incorporated in τ. We see from Eq. (3) that, due to the small thickness of the conductor, the lateral dispersion introduces a competitive time scale, which influences the evolution of θ. In the limits of high radius, ($r\to\infty$), or isolated wire, ($\sigma=0$), namely, as $\tau_r\to\infty$, Eq. (3) reduces to the classical telegraph equation arising in Maxwell–Cattaneo–Vernotte theory.

In Fig. 1 we plot at different scales the ratio τ/τ_r in a silicon nanowire, as a function of the temperature, for two different values of the radius. We see that in the range of temperatures from 100 K to 300 K, τ is of the order of $10^{-5}\tau_r$. Hence, in Eq. (3) the term $\dot{\theta}/\tau$ is predominant with respect to $\dot{\theta}/\tau_r$. In the range from 30 K to 100 K, instead, τ may be of the order of $10^{-3}\tau_r$, so that the influence of $\dot{\theta}/\tau_r$ on the solution of Eq. (3) may be relevant.

Let us put our attention now on the propagation of plane temperature-waves

$$\theta(x;t)=\bar{\theta}_0\exp\bigl[i(\omega t-\kappa x)\bigr], \tag{6}$$

which may be experimentally realized by imposing at one end of the system a sinusoidally time-dependent temperature, and calculating the consequent temperature perturbation at different points along the system [27,28].