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Focusing of heat pulses along nonequilibrium nanowires

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ABSTRACT

As a consequence of the temperature dependence of the speed of heat pulses, rectangular heat pulses will shrink (or extend) spatially, and will increase (or decrease) their temperature when propagating along a temperature gradient. Here, we consider heat pulse propagation along silicon nanowires, because of their interest in nanotechnology. The relative rates of variation per meter may be very high, and variations along relatively short lengths could be experimentally observable.

1. Introduction

Heat pulses propagate at a speed given by the high-frequency limit of phase speed of thermal waves. In the classical theory, where heat transport is described by the Fourier law, this velocity diverges [1–6]. When relaxational effects are incorporated to the heat transport equation, instead, this speed becomes finite, in agreement with experimental observations [7–11]. A further step in the analysis of energy pulses and thermal waves is to study their propagation in a nonequilibrium steady state characterized by a nonvanishing temperature gradient, or heat flux, to explore their change of speed and form when the pulse travels along or against the temperature gradient. This is a nontrivial problem, because dealing with it requires the incorporation of nonlinear terms in the transport equation, and such terms are not well known.

The aim of the present work is to explore how a rectangular energy pulse evolves along its propagation in a nonequilibrium steady state. The basic idea is simple: since the propagation speed of an energy pulse depends on temperature, and since the temperature may vary along the system, the two boundaries of the energy pulse will propagate with slightly different speeds. This will make that the energy pulse shrinks, when the frontal border x_f is slower than the rear border x_r (Fig. 1(a)), namely, the initial width of the pulse Δx_0 reduces along the propagation. In the opposite case, instead, the energy pulse will enlarge along the propagation (Fig. 1(b)). Because of energy conservation, if the pulse shrinks its temperature will rise, or reciprocally in the opposite situation. Indeed, its total internal energy I will be proportional to the product of its temperature amplitude $\Delta\theta = (\theta_{\max} - \theta_{\mathrm{avg}})$ times its width Δx, namely, $I \propto c_v \Delta\theta \Delta x$, being c_v the specific heat per unit volume, $\theta_{\max}$ the maximum temperature of the pulse, and θ_{avg} the average temperature of the system. From a practical point of view, increasing in temperature may lead to a temperature higher than the fusion threshold of the material, and thus the breaking point of the nanowire could be reached. This justifies the interest in analyzing this effect in detail by exploring, for instance, the rate of temperature variation of the pulse, in order to explore how it depends on the material and on the direction of propagation relative to the temperature gradient.

In Section 2 we briefly introduce and discuss the nonlinear heat transport equations, and in Section 3 we concentrate our attention on the rate of variation of the height and width of the heat pulse both in the case of a thin wire and in the case of a nanowire. The

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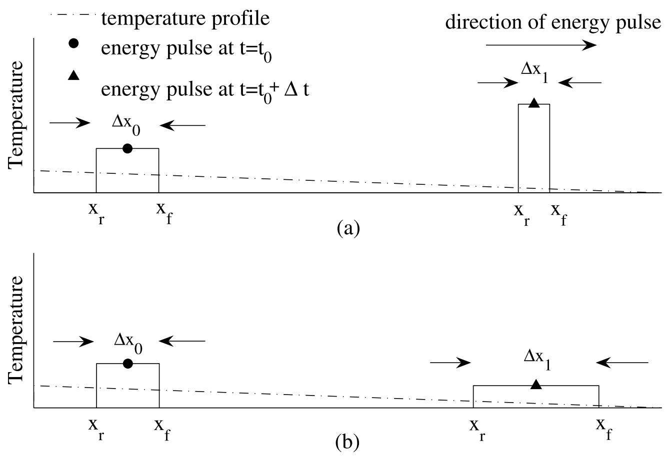

Fig. 1. Figures show the possible evolutions of a rectangular energy pulse. It is supposed to travel from left to right. If the speed of propagation of the energy-pulse frontal border (x_f) is slower than that of the rear border (x_r), the pulse spatially shrinks and increases its temperature (a). Conversely, if the speed of propagation of the energy-pulse frontal border is faster than that of the rear border, then the pulse spatially enlarges and decreases its temperature (b).

nanowire we analyze is made by silicon with an average temperature varying from 30 K to 200 K.

2. Generalized heat transport equation

Starting from the idea of a heat flux $\mathbf{q}$ proportional to the gradient of the dynamical semiempirical temperature β [12,13], namely, $\mathbf{q} = -\lambda \nabla \beta$ with λ as the bulk thermal conductivity, in Ref. [6] it has been obtained the following nonlocal evolution equation for β

$$\dot{\beta} = -\frac{1}{\tau}(\beta - \theta) - \frac{\chi}{\theta} \nabla \beta \cdot \nabla \beta, \tag{1}$$

for constant material functions $\chi = \lambda / c_v$ (representing the thermal diffusivity) and the relaxation time τ (which may be linked, for instance, to resistive processes of interaction among the phonons, representing the heat carriers). Moreover in Eq. (1) θ means the thermodynamic absolute nonequilibrium temperature, and a superposed dot indicates the time derivative of its argument. The physical meaning of β has been discussed at length in Refs. [6, 12,13]. It is related to the disordered contribution of the molecular energy to the internal energy of the system; in equilibrium, and at rest, all the molecular energy is disordered; however, during fast changes of the state a fraction of the energy is flowing from some microscopic states to others in an organized way during a short time, until the final local-equilibrium state is reached. A comparison between the definitions of θ and β and their consequences on the propagation of thermal waves in nanosystems has been performed by Jou et al. [14].

Before going further, it seems important to underline that in the present Letter we will restrict ourselves to second-order nonlinear terms in the heat flux in the transport equations. Higher-order terms, as those following, for instance, from the fourth power in $\nabla \beta$ in Eq. (1), or terms like $\dot{\theta}\theta_{,i} q_i$ and $\dot{\beta}\theta_{,i}^2$ in Eq. (3) of Section 3 will be neglected. This implies that the heat flux is not too high, namely, the heat flux $\mathbf{q}$ is considerably smaller than the specific internal energy (estimated as the product of the specific heat times the temperature) times the propagation speed of heat pulses.

The combination of the constitutive assumption $\mathbf{q} = -\lambda \nabla \beta$ with the gradient of Eq. (1) leads to a relaxational and nonlinear transport equation for $\mathbf{q}$, given by

$$\tau \dot{\mathbf{q}} + \mathbf{q} = -\lambda \nabla \theta + \frac{2}{\theta} \frac{\tau}{c_v} \mathbf{q} \cdot \nabla \mathbf{q}, \tag{2}$$

which incorporates both relaxation terms (characterized by τ), and nonlinear terms. In the absence of nonlinear terms, it becomes the well-known Maxwell–Cattaneo equation [1–6] leading to finite speed $U_0 = \sqrt{\chi/\tau}$ for propagation of heat pulses. When the relaxation time vanishes this equation reduces to the Fourier equation, which predicts, instead, divergent speed for heat pulses. This divergence refers to the speed of high-frequency small-amplitude thermal waves. Fourier law admits finite-speed propagation for some nonlinear – i.e., high amplitude – signals [15,16]. In this Letter, we refer to the propagation of high-frequency small-amplitude waves along a nonequilibrium steady state characterized by an average nonvanishing heat flux. Of course, when the frequency is very high, the influence of a nonvanishing relaxation time, as expressed in the first an the last terms of Eq. (2) cannot be neglected. We will study this influence. The combination of these effects and the nonlinear effects of Fourier equation would be especially interesting, but it refers to the propagation of high-amplitude waves, and we will not consider it here.

Let us finally note that Chen [11] has also incorporated the nonvanishing relaxation time τ in a ballistic-diffusive model for heat transport. In his work, he splits the total phonon population in a ballistic group and a diffusive group, and the Cattaneo equation is applied to the former one. Here, instead, we will consider a single population but with an effective thermal conductivity (see Eq. (13) of Section 3) which takes into account the relative proportion of ballistic versus diffusive phonons. Moreover, Chen's equation does not contain the last term of the right-hand side in Eq. (2), which goes beyond the Cattaneo equation. The presence of this term is, instead, in accordance with the results by Grmela et al. [17], where the thermodynamic compatibility of Chen's model has been investigated in the light of the GENERIC approach to nonequilibrium thermodynamics [18]. They found that Cattaneo equation is modified by five additional terms in the heat flux. One of the new terms, namely, the one that appears also in Chen's theory, is the additional energy flux due to the ballistic heat conduction. The remaining four terms are nonlinear functions of quantities that disappear at equilibrium. The same is true for the nonlinear term in Eq. (2) which disappears at the equilibrium, since in such a situation the states are necessarily homogeneous, i.e., $\nabla \mathbf{q} = 0$. Note that the nonlinear term in Eq. (2) has been not introduced to make Cattaneo equation compatible with second law of thermodynamics. A supposed violation of second law by Cattaneo equation is known in the literature as Taitel Paradox [19–21]. However, as proved by Sharma [15], this is due to unrealistic initial time conditions. The paradox is removed if more realistic initial conditions are given. The nonlinear term in Eq. (2) is, instead, a direct consequence of the evolution equation for β [Eq. (1)], where the appearance of $\nabla \beta$ accounts for nonlocal effects, which become important in miniaturized systems whose physical dimension is smaller than mean-free path of the heat carriers.

A derivation analogous to Eq. (2) may be found in the framework of extended irreversible thermodynamics (EIT), a macroscopic theory in which the heat flux, and other possible fluxes, are considered as independent variables contributing to the entropy. The contribution of the fluxes may be derived from several bases, as for instance the kinetic theory of gases or the fluctuation–dissipation theory [1,2,22]. It is also worth noticing the transport equation obtained by Coleman and Owen [23]. Anyway, all these equations lead to qualitatively analogous solution that heat waves, in the presence of a temperature gradient, propagate at different velocities along or against the temperature gradient [6,22,24].

3. Heat waves propagation in nonequilibrium steady states

Taking into account the hypothesis $\mathbf{q} = -\lambda \nabla \beta$, a further alternative description to the Maxwell–Cattaneo equation with respect