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Macroscopic heat transport equations and heat waves in nonequilibrium states

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HIGHLIGHTS

- A generalized heat transport equation including nonlinear, nonlocal and relaxation terms is proposed.
- Heat wave propagations are investigated systematically in nonequilibrium steady states.
- The phase (or front) speed of heat waves is intimately related to the nonlinear and nonlocal terms.

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ABSTRACT

Heat transport may behave as wave propagation when the time scale of processes decreases to be comparable to or smaller than the relaxation time of heat carriers. In this work, a generalized heat transport equation including nonlinear, nonlocal and relaxation terms is proposed, which sums up the Cattaneo–Vernotte, dual-phase-lag and phonon hydrodynamic models as special cases. In the frame of this equation, the heat wave propagations are investigated systematically in nonequilibrium steady states, which were usually studied around equilibrium states. The phase (or front) speed of heat waves is obtained through a perturbation solution to the heat differential equation, and found to be intimately related to the nonlinear and nonlocal terms. Thus, potential heat wave experiments in nonequilibrium states are devised to measure the coefficients in the generalized equation, which may throw light on understanding the physical mechanisms and macroscopic modeling of nanoscale heat transport.

1. Introduction

Heat waves contribute to heat transport in fast processes besides the usual diffusive transport described by Fourier's law, and on the other hand, they may provide new experimental tools for the analysis of physical systems [1–10]. Recent investigations of heat transport in carbon nanotubes [11–13] and in graphene sheets or nano-ribbons [14–16] have declared the role of several non-Fourier features, related to a combined heat transfer in diffusive form and in form of heat waves. For instance, in Ref. [14] the authors studied the effects of a rapid cooling of four layers of carbon atoms at one end of a graphene nano-ribbon, which leads to rapid propagation of thermal perturbation, especially at the early period. They observed temperature responses described by the following generalized heat transport equation:

$$\frac{1}{\alpha}\frac{\partial T}{\partial t}+\frac{\tau_q}{\alpha}\frac{\partial^2 T}{\partial t^2}=\nabla^2 T+\tau_\theta\frac{\partial}{\partial t}\left(\nabla^2 T\right), \tag{1}$$

with α the thermal diffusivity, and τ_q and τ_θ two phase lags. In particular, they found $\tau_q = 1.85$ ps, $\tau_\theta = 1.01$ ps and $\alpha = 1.44 \times 10^{-5}$ m^2/s for a ribbon of length 14.9 nm. Although these values are very small, they are measurable by current experimental techniques. This work is mentioned as an example of generalized heat transport equations not only beyond Fourier's law ($\tau_q = \tau_\theta = 0$) but also beyond Cattaneo–Vernotte (C–V) law [17,18] ($\tau_\theta = 0$), one of the well-known equations in the description of heat waves [1,7]. The need to go beyond C–V law in the analysis of actual fast thermal processes motivates the current interest in exploring generalized heat transport equations.

In the present work, a generalized heat transport equation is proposed, which incorporates nonlinear and nonlocal terms into

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the C–V law. It sums up many previous macroscopic models for nanoscale heat transport [9] as special cases, allowing a comparison between their respective physical consequences in the propagation of heat waves. Usually, heat wave propagation was studied around equilibrium states [11–16,19–22]. Propagation of heat waves in nonequilibrium steady states has been only considered for some particular cases [23–28]. However, the nonlinear terms often neglected in generalized heat transport models have an intimate relevance to wave propagation in nonequilibrium steady states [26–28]. Thus the present work generalizes much the few previous works on this issue, and gives rise to some new features of heat waves along nonequilibrium steady states based on the proposed generalized equation. In addition, nanotechnology opens new perspectives to this problem, because it becomes possible to study the speed of thermal perturbations along carbon nanotube or graphene ribbons with their ends kept at different temperatures, thus imposing a controlled non-vanishing average heat flux along them.

The remainder of this article is organized below. In Section 2, the generalized heat transport equation is introduced, with a summary of how one may recover from it diverse heat transport equations of existing macroscopic models. Besides, the kinetic theory and thermodynamic foundations are also discussed for the generalized heat transport equation. In Section 3, the influences of nonlinear and nonlocal terms in the generalized equation are systematically studied on the phase speed of heat waves or front speed of heat pulse perturbations around nonequilibrium steady state. In Sections 4 and 5, discussions and concluding remarks are made.

2. A generalized heat transport equation

A generalized heat transport equation including nonlinear and nonlocal terms as well as a relaxation term is proposed as:

$$\tau\frac{\partial\mathbf{q}}{\partial t}+\mathbf{q}=-\lambda\nabla T+m_1\mathbf{q}\nabla\cdot\mathbf{q}+m_2\mathbf{q}\cdot\nabla\mathbf{q}+m_3\nabla\mathbf{q}^2+m_4\nabla^2\mathbf{q}+m_5\nabla(\nabla\cdot\mathbf{q})+m_6\mathbf{q}(\mathbf{q}\cdot\nabla T)+m_7\mathbf{q}^2\nabla T, \tag{2}$$

where τ is the relaxation time of heat flux, λ is the thermal conductivity, and $m_i(T)$ ($i = 1,2,\dots,7$) are temperature dependent coefficients to be identified below. In physical views, the main motivation in incorporating these terms originates in the analysis of nanosystems, where the spatial gradients of physical quantities such as temperature and heat flux may be extremely large due to the minute size of the system. On the other hand, the temporal derivative of heat flux may be extremely high in the fast local heating of a sample by intense and narrow laser beams. Eq. (2) contains particular cases of many previous macroscopic models for nanoscale heat transport, and provides a common ground for a comparison between them.

To recover the classical Fourier's law, all the terms in τ and m_i are vanishing whereas for the C–V law only the relaxation term is kept. The coefficients m_i are identified through comparing Eq. (2) to the heat transport equations respectively in dual-phase-lag (DPL) model [10]:

$$\tau_q\frac{\partial\mathbf{q}}{\partial t}+\mathbf{q}=-\lambda\nabla T-\lambda\tau_T\frac{\partial}{\partial t}(\nabla T), \tag{3}$$

with τ_q, τ_T the phase lags of heat flux and temperature gradient, in Guyer–Krumhansl (G–K) model [29] (phonon hydrodynamics model [30]):

$$\tau_R\frac{\partial\mathbf{q}}{\partial t}+\mathbf{q}=-\lambda\nabla T+l^2\left[\nabla^2\mathbf{q}+2\nabla(\nabla\cdot\mathbf{q})\right], \tag{4}$$

with $l^2=\tau_N\tau_R v_g^2/5$, τ_N, τ_R the relaxation times of phonon normal (N) and resistive (R) processes and v_g the average phonon group speed, in the nonlinear G–K model [28]:

$$\tau_R\frac{\partial\mathbf{q}}{\partial t}+\mathbf{q}=-\lambda\nabla T+\frac{2}{T}\frac{\tau_R}{C_V}\mathbf{q}\cdot\nabla\mathbf{q}+l^2\left[\nabla^2\mathbf{q}+2\nabla(\nabla\cdot\mathbf{q})\right], \tag{5}$$

with C_V the heat capacity per unit volume, and in the thermon gas model [31,32]:

$$\tau_T\frac{\partial\mathbf{q}}{\partial t}+\mathbf{q}=-\lambda\nabla T-\frac{\tau_T}{C_VT}\mathbf{q}\nabla\cdot\mathbf{q}-\frac{\tau_T}{C_VT}\mathbf{q}\cdot\nabla\mathbf{q}+\frac{\tau_T}{C_VT^2}\mathbf{q}(\mathbf{q}\cdot\nabla T), \tag{6}$$

with τ_T the relaxation time of thermon gas. Note that to recover Eq. (3) in the DPL model, the energy balance equation is supplemented [6]:

$$C_V\frac{\partial T}{\partial t}=-\nabla\cdot\mathbf{q}, \tag{7}$$

and the mixed partial derivative of temperature in Eq. (3) is reformulated as:

$$\frac{\partial}{\partial t}(\nabla T)=\nabla\left(\frac{\partial T}{\partial t}\right)=-\frac{1}{C_V}\nabla(\nabla\cdot\mathbf{q}). \tag{8}$$

The relations between the coefficients in Eq. (2) and those in the previous heat transport models are thoroughly summarized in Table 1. Besides, the terms in Eq. (2) with coefficients m_3 and m_7 not explicitly correlated to previous models could be got from a nonequilibrium temperature θ dependent on heat flux. The nonequilibrium temperature is obtained in extended irreversible thermodynamics as $\theta^{-1}\equiv\partial s/\partial u$ with $s\equiv s(u,\mathbf{q})$ a generalized entropy dependent on u and $\mathbf{q}$, and becomes [6]:

$$\theta^{-1}=T^{-1}-\frac{1}{2}\frac{\partial}{\partial u}\left(\frac{\tau}{\rho\lambda T^2}\right)\mathbf{q}\cdot\mathbf{q}. \tag{9}$$

Substitution of Eq. (9) into an extended Fourier's law $\mathbf{q}=-\lambda\nabla\theta$ with an approximation $\theta\approx T+\xi(T)\mathbf{q}^2$ ($\xi(T)\equiv\frac{1}{2}T^2\partial\left(\tau/\rho\lambda T^2\right)/\partial u$ for brevity) gives rise to:

$$\mathbf{q}=-\lambda\left(1+\frac{\partial\xi}{\partial T}\mathbf{q}^2\right)\nabla T-\lambda\xi\nabla\mathbf{q}^2. \tag{10}$$

Thus the coefficients are identified as: $m_7=-\lambda\partial\xi/\partial T$, and $m_3=-\lambda\xi$. The terms in m_3 and m_7 could be logically incorporated as additional terms into the nonlinear G–K model equation (5) through the temperature gradient term, but usually they are not considered for simplicity because of their negligible effect.

Therefore the generalized heat transport equation (2) contains in a compact way the heat transport equations of diverse previous macroscopic models. Furthermore, these terms with coefficients m_i in Eq. (2) are not merely written in a phenomenological way, but actually deeply rooted in the kinetic theory of phonons [33,34]. The following heat transport equation has been derived from phonon Boltzmann equation by either maximum entropy [35] or Grad's type [36] moment methods and Chapman–Enskog expansion within zeroth-order approximation [9,37]:

$$\tau_R\frac{\partial\mathbf{q}}{\partial t}+\mathbf{q}=-\lambda\nabla T-\frac{3\tau_R}{C_V}\nabla\cdot\frac{\langle\mathbf{q}\mathbf{q}\rangle}{2T\left[1+\sqrt{1-\frac{3}{4}\left(q/v_gC_VT\right)^2}\right]}, \tag{11}$$

where the deviatoric part of the tensor $\mathbf{q}\mathbf{q}$ denotes $\langle\mathbf{q}\mathbf{q}\rangle=\mathbf{q}\mathbf{q}-\frac{1}{3}\mathbf{q}^2\mathbf{I}$, with $\mathbf{I}$ the unit tensor. For relatively small heat flux ($q/v_gC_VT\ll 1$), Eq. (11) is approximated as:

$$\tau_R\frac{\partial\mathbf{q}}{\partial t}+\mathbf{q}=-\lambda\nabla T-\frac{3\tau_R}{4C_V}\nabla\cdot\frac{\langle\mathbf{q}\mathbf{q}\rangle}{T}. \tag{12}$$