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From Boltzmann transport equation to single-phase-lagging heat conduction

Lin Cheng [a], Mingtian Xu [a,*], Liqiu Wang [b]

[a] Institute of Thermal Science and Technology, Shandong University, P.O. Box 88, Jing Shi Road 73, Jinan, Shandong Province, PR China
[b] Department of Mechanical Engineering, University of Hong Kong, Pokfulam Road, Hong Kong

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ABSTRACT

In the present work the single-phase-lagging heat conduction model is re-derived analytically from the Boltzmann transport equation. In contrast to the Maxwell–Cattaneo law (CV model), it is Galilean invariant in the moving media. Based on this model, the governing equation of the microscale heat conduction is established, which is formulated into a delay partial differential equation. The corresponding initial and boundary conditions are prescribed. The thermal oscillation of the single-phase-lagging heat conduction is investigated.

1. Introduction

Consider the classical Fourier law in a homogeneous and isotropic thermally conducting medium

$$\mathbf{q}(\mathbf{r},t) = -k\nabla T(\mathbf{r},t), \tag{1}$$

where the temperature gradient $\nabla T(\mathbf{r},t)$ is a vector function of the position vector $\mathbf{r}$ and the time variable t, the vector $\mathbf{q}(\mathbf{r},t)$ is called the heat flux, k is the thermal conductivity of the material. This classical law has been widely and successfully applied to the conventional engineering heat conduction problems, in which the system has large spatial dimension and the emphasis is on the long time behavior. However, it leads to the infinite speed of heat propagation, implying that a thermal disturbance applied at a certain location in a heat conduction medium can be sensed immediately anywhere else in the medium. This is unaccepted in the transient behavior at extremely short time, say, on the order of picoseconds to femtoseconds. An example is the ultrafast laser heating in thermal processing of materials.

Experimentally it is also shown that the propagation of second sound, ballistic phonon propagation and phonon hydrodynamics in solids at low temperatures depart significantly from the usual parabolic description [1]. With the advances of modern microfabrication technology, more and more microdevices with micro- and nano-scale dimension emerge in various micromechanical systems. The understanding of the microscale heat transport phenomena is critical for the further development of the nanotechnology, especially for the cooling of the large scale integrate circuit. However, the traditional Fourier law leads to the unaccepted result for the microscale heat conduction [2–4]. Many phenomena in the discrete systems including the low-dimensional lattices also challenge the validity of the classical Fourier law [5–7].

Much effort has already been devoted to the modification of the classical Fourier law, which leads to many non-Fourier laws. The most famous one among them is the CV model proposed by Cattaneo and Vernotte [8–10]:

$$\tau\frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -k\nabla T, \tag{2}$$

where τ is the time delay. The CV model gives rise to a wave type of heat conduction equation called the hyperbolic heat conduction equation [11]. The natural extension of this model is

$$\mathbf{q}(\mathbf{r},t+\tau) = -k\nabla T(\mathbf{r},t), \tag{3}$$

which was proposed by Tzou [12–16]. The constitutive relation (3) is called the single-phase-lagging (SPL) heat conduction model. The model (3) was further extended to the dual-phase-lagging (DPL) model by Tzou and formulated mathematically as follows [1,17–19]:

$$\mathbf{q}(\mathbf{r},t+\tau_q) = -k\nabla T(\mathbf{r},t+\tau_T), \tag{4}$$

where τ_T and τ_q are the phase lags of the temperature gradient and the heat flux vector, respectively. The first order Taylor expansion of Eq. (4) gives

$$q(\mathbf{r},t) + \tau_q\frac{\partial \mathbf{q}}{\partial t}(\mathbf{r},t) \cong -k\left\{\nabla T(\mathbf{r},t) + \tau_T\frac{\partial}{\partial t}[\nabla T(\mathbf{r},t)]\right\}, \tag{5}$$

which leads to the following governing equation of the temperature field:

$$T_t(\mathbf{r},t) + \tau_q T_{tt}(\mathbf{r},t) = \alpha(\Delta T(\mathbf{r},t) + \tau_T\Delta T_t(\mathbf{r},t)), \tag{6}$$

where the subscript t indicates the partial derivative with respect to time.

* Corresponding author. Tel.: +86 531 99595 6503.
E-mail address: mingtian@sdu.edu.cn (M. Xu).

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Nomenclature

f	distribution function
k	thermal conductivity
$\mathbf{r}$	position vector
$\mathbf{q}$	heat flux
t	time variable
T	temperature field
$\mathbf{v}$	velocity vector

Greek symbols

τ	relaxation time
τ_q	phase lag of the heat flux vector
τ_T	phase lag of the temperature gradient

Eq. (6) plays a significant role in the investigation of the microscale heat conduction. Firstly it is a unified form of the energy equations of the phonon–electron interaction model [20] and the phonon scattering model [11,21]. These two models have been developed in examining energy transport involving the high-rate heating in which the non-equilibrium thermodynamic transition and the microstructural effect become important associated with shortening of the response time [1,22]. The high-rate heating is developing rapidly due to the advancement of high-power short-pulse laser technologies [23–27]. In addition to its application in the ultrafast pulse-laser heating, the microscale heat conduction equation (6) also arises in describing and predicting phenomena such as temperature pulses propagating in superfluid liquid helium, nonhomogeneous lagging response in porous media, thermal lagging in amorphous materials, and effects of material defects and thermo-mechanical coupling, etc. [1]. The study of Eq. (6) is thus of considerable importance in understanding and applying these rapidly emerging technologies. We have examined its well-posedness [28,29] and investigated the thermal oscillation and resonance phenomena in detail [30] which are believed to be a manifestation of non-equilibrium behavior of microscale heat conduction [22].

Unfortunately, it was shown that the CV model violates the Galilean principle of relativity [31], thus it cannot be applied to the moving medium. Therefore, it is desirable to examine whether the model (3) suffers from the same drawback.

The Boltzmann transport equation (BTE) is a fundamental equation in statistical physics for describing the non-equilibrium phenomena. Therefore, many efforts are dedicated to establishing the non-Fourier laws from the BTE. The phonon–electron interaction model [20] was developed from BTE on a quantum mechanical and statistical basis. A phonon radiative transport equation between two parallel plates was established from the BTE for the heat transport in dielectric solid films [3]. Based on the BTE, Chen [32,33] proposed a ballistic–diffusive heat conduction model of microscale heat transport in devices where the characteristic length is comparable to the mean free path of the energy-carrier and/or the characteristic time is comparable to the relaxation time of the energy-carrier. The classical Fourier law and CV model were also re-established from the BTE [4]. Recently, we re-derived the dual-phase-lagging heat conduction model (4) from the discrete form of the BTE [34]. In the present work the methodology in [34] is developed to re-establish the SPL heat conduction model (3) from the BTE in the partial differential equation form.

Finally, the governing equation of the SPL heat conduction, which is expressed as the delay partial differential equation, is obtained by combining Eq. (3) with the energy balance equation. The associated initial and boundary conditions for this equation are prescribed. The thermal oscillation phenomenon is investigated.

2. Examination of SPL model by Galilean principle of relativity

In [31], it was found that the CV model is not Galilean invariant. In this section we attempt to examine the SPL model (3). Consider the following Galilean transformation and some notations:

$$\mathbf{r}' = \mathbf{r} - \mathbf{U}t, \quad t = t, \quad \theta(\mathbf{r}', t) = T(\mathbf{r}', t), \quad \mathbf{q}'(\mathbf{r}', t) = \mathbf{q}(\mathbf{r}', t), \tag{7}$$

where $\mathbf{U}$ is the constant velocity between two inertial reference frames. From the first relation in Eq. (7), it is evident that $\nabla_{\mathbf{r}'} = \nabla_{\mathbf{r}}$. Therefore, we have

$$\nabla_{\mathbf{r}'}\theta(\mathbf{r}', t) = \nabla_{\mathbf{r}} T(\mathbf{r}, t). \tag{8}$$

Subsequently, Eq. (3) becomes

$$\mathbf{q}'(\mathbf{r}', t + \tau) = -k\nabla_{\mathbf{r}'}\theta(\mathbf{r}', t). \tag{9}$$

The observation shows that Eq. (9) has the same form as Eq. (3) and it does not involve the velocity $\mathbf{U}$. Thus the SPL heat conduction model is invariant under the Galilean transformation (7) and can be employed to study the microscale heat conduction problems in moving media. Therefore, compared with the CV model, it has the obvious advantage.

Note that the first order Taylor expansion of the left side of Eq. (3) with respect to the time variable gives rise to the CV model (2) which violates the Galilean principle of relativity. Then one natural question is whether the higher order approximation of the left side of Eq. (3) would lead to the Galilean invariant heat conduction models. In order to address this question, we first consider the following heat conduction model with the lagging behavior:

$$\mathbf{q}(\mathbf{r}, t) + \tau\frac{\partial \mathbf{q}(\mathbf{r}, t)}{\partial t} + \frac{\tau^2}{2}\frac{\partial^2 \mathbf{q}(\mathbf{r}, t)}{\partial t^2} = -k\nabla T, \tag{10}$$

which is obtained by the second order approximation of the left side of Eq. (3). By the Galilean transformation (7), we have

$$\frac{\partial \mathbf{q}(\mathbf{r}, t)}{\partial t} = \frac{\partial \mathbf{q}'(\mathbf{r}', t)}{\partial t} - \frac{\partial \mathbf{q}'(\mathbf{r}', t)}{\partial \mathbf{r}'}\cdot \mathbf{U}, \tag{11}$$

$$\frac{\partial^2 \mathbf{q}(\mathbf{r}, t)}{\partial t^2} = \frac{\partial^2 \mathbf{q}'(\mathbf{r}', t)}{\partial t^2} - 2\frac{\partial^2 \mathbf{q}'(\mathbf{r}', t)}{\partial t \partial \mathbf{r}'}\cdot \mathbf{U} + \mathbf{U}\cdot\frac{\partial^2 \mathbf{q}'(\mathbf{r}', t)}{\partial^2 \mathbf{r}'}\cdot \mathbf{U}. \tag{12}$$

Substituting Eqs. (8), (11) and (12) into Eq. (10) yields

$$\mathbf{q}'(\mathbf{r}', t) + \tau\left[\frac{\partial \mathbf{q}'(\mathbf{r}', t)}{\partial t} - \frac{\partial \mathbf{q}'(\mathbf{r}', t)}{\partial \mathbf{r}'}\cdot \mathbf{U}\right] + \frac{\tau^2}{2}\left[\frac{\partial^2 \mathbf{q}'(\mathbf{r}', t)}{\partial t^2} - 2\frac{\partial^2 \mathbf{q}'(\mathbf{r}', t)}{\partial t \partial \mathbf{r}'}\cdot \mathbf{U} + \mathbf{U}\cdot\frac{\partial^2 \mathbf{q}'(\mathbf{r}', t)}{\partial^2 \mathbf{r}'}\cdot \mathbf{U}\right] = -k\nabla_{\mathbf{r}'}\theta(\mathbf{r}', t). \tag{13}$$

Note that Eq. (13) depends on the constant velocity $\mathbf{U}$. This indicates that the constitutive relation (10) is not independent on the observer's speed, therefore, violates the Galilean principle of relativity. Similar deductions show that the other higher order approximations of the SPL heat conduction model (3) suffer from the same drawback. From the above derivation, one can see that it is the presence of the time partial derivative in the constitutive relation that leads to the violation of the Galilean principle of relativity.

3. Boltzmann transport equation and SPL model

3.1. Boltzmann transport equation

In the absence of external forces, the Boltzmann transport equation reads