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Dual-phase-lagging heat conduction based on Boltzmann transport equation

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

[a] Forschungszentrum Rossendorf, P.O. Box 510119, D-01314 Dresden, Germany
[b] Department of Mechanical Engineering, The University of Hong Kong, Hong Kong

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Abstract

In this work, the dual-phase-lagging model of the microscale heat conduction is re-derived analytically from the Boltzmann transport equation. Based on this model, the delay/advanced partial differential equations governing the microscale heat conduction are established. The method of separation of variables is applied to solve such delay/advanced partial differential equations. Finally, the oscillation of the microscale heat conduction is investigated.

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1. Introduction

It has a long history to explore the macroscopic properties from the molecular level of description of the materials. This coarse-graining process allows us to bridge the gap between microscopic and meso/macroscopic descriptions. The understanding of coarse-graining and its correlated theories such as transport processes and irreversible phenomena was strengthened in the middle of last century by people like Kirkwood [12], Green [7], Kubo [15], Zwanzig [33–35] and many others. Recently, the rapid development of nano-technology gives a new impetus to this old topic. In the present work, we attempt to re-derive the dual-phase-lagging model of microscale heat conduction starting from the molecular level of description, the Boltzmann transport equation.

The fundamental law of the conventional heat conduction is the classical Fourier law

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

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 which is a positive scalar quantity. This classical law has been widely and successfully applied in the conventional engineering heat conduction problems, in which the system has large spatial dimension and the emphasis is on the long time behavior. However, the Fourier law suffers some drawbacks. Firstly, it assumes the infinite speed of heat propagation, implying that a thermal disturbance applied at a certain location in a medium can be sensed immediately anywhere else in the medium. Secondly, because the heat flux and the temperature gradient are simultaneous, there is no difference between the cause and the effect of heat flow. This is doubted 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. Thirdly, experimental observations of heat transport of the

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[*] Corresponding author.
E-mail address: M.Xu@fz-rossendorf.de (M. Xu).

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Nomenclature

f	distribution function
k	thermal conductivity
$\mathbf{r}$	position vector
$\mathbf{q}$	heat flux
t	time vector
T	temperature field
$\mathbf{v}$	velocity vector
Greek symbols	
τ	relaxation time
τ_q	the phase lag of the heat flux vector
τ_{T}	the phase lag of the temperature gradient

propagation of second sound, ballistic phonon propagation and phonon hydrodynamics in solids at low temperatures depart significantly from the usual parabolic description. Furthermore, due to the wide application of microdevices and the rapid development of modern microfabrication technology, more and more microdevices with micro and nano-scale dimension emerge in various micromechanical systems. It is well known that the conventional Fourier law leads to the unaccepted result for these microdevices [11].

Many efforts have been spent on the improvement of classical Fourier law. Cattaneo [3] and Vernotte [28,29] proposed the CV model,

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

where τ is the time delay. This leads to a wave type of heat conduction equation called hyperbolic heat conduction equation [10]. The natural extension of CV model is

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

which was discussed in Tzou [19–23]. Further improvement of the model (3) leads to the dual-phase-lagging (DPL) model by Tzou [27]. It allows either the temperature gradient (cause) to precede the heat flux vector (effect) or the heat flux vector (cause) to precede the temperature gradient (effect) in transient processes. Mathematically, this is represented by [24–27]

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

where the τ_{T} is the phase lag of the temperature gradient and the τ_q is the phase lag of the heat flux vector. For the case of $\tau_{\mathrm{T}}>\tau_q$, the temperature gradient established across a material volume is a result of the heat flow, implying that the heat flux vector is the cause and the temperature gradient is the effect. For $\tau_{\mathrm{T}}<\tau_q$, on the other hand, heat flow is developed by the temperature gradient established at an earlier time, implying that the temperature gradient is the cause. The first-order approximation of Eq. (4) reads

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

In the literatures, the dual-phase-lagging (abbreviated as DPL) model usually refers to this model. However, in the present paper, we mainly focus on the original DPL model expressed in (4).

Originally, the DPL heat conduction equation comes from the phonon–electron interaction model [17] and the phonon scattering model [8,10]. These 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. The high-rate heating is developing rapidly due to the advancement of high-power short-pulse laser technologies [1,6,13,14,16]. In addition to its application in the ultrafast pulse laser heating, the DPL heat conduction equation also arises in describing and predicting phenomena such as temperature pulses propagating in superfluid liquid helium, non-homogeneous lagging response in porous media, thermal lagging in amorphous materials, and effects of material defects and thermomechanical coupling etc. [27]. The study of the DPL heat conduction is thus of considerable importance in understanding and applying these rapidly emerging technologies. The well-posedness of DPL heat conduction was established [30,31]. The thermal oscillation and resonance phenomena were investigated in detail by Xu and Wang [32] based on the approximate DPL model (5). Such phenomena are believed to be a manifestation of non-equilibrium behavior of microscale heat conduction. The Boltzmann transport equation (BTE), a theory of non-equilibrium heat and mass transport, may therefore be useful for examining the microscale heat conduction.

Indeed, the BTE is playing a central role in the study of microscale heat conduction. The classical Fourier law and the CV model for one-dimensional case was established from the BTE [18]. The phonon–electron interaction model [17] was derived from BTE on a quantum mechanical and statistical basis. Joshi and Majumdar [11] derived a phonon radiative transport equation between two parallel plates from the BTE for the heat transport in dielectric solid films. Based on the BTE, Chen [4,5] proposed a ballistic–diffusive heat conduction equation 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. Encouraged by the successful applications of BTE in the microscale heat conduction, we attempt to establish the DPL model (4) from the BTE. The governing equation of DPL heat conduction, which is expressed as the delay/advanced partial differential equations, is then obtained by combining the DPL heat conduction model with the energy conservation equation. The associated initial conditions for this equation is prescribed. The method of separation of variables is employed to solve the DPL heat conduction problems. The oscillating features of microscale heat conduction are also investigated.

2. Boltzmann transport equation and DPL model

2.1. Boltzmann transport equation

Consider a classical system of N particles. Each particle has s degrees of freedom so that the number of coordinates needed to specify positions of all N particles is $l = Ns$. Therefore l spatial coordinates q_i and l corresponding velocity coordinates v_i can completely describe the classical mechanical state of the system. We now introduce a conceptual Euclidean hyperspace of $2l$ dimensions, with a coordinate axis for each of the $2l$ coordinates and velocities. This conceptual space is usually termed as the phase space for the system. The state of the classical N-particle or N-body system at any time t is completely specified by the location of one point in the phase space, referred to as a phase point. The evolution of the system state with time is completely described by the motion or trajectory of the phase point through phase space. The trajectory of the point is expressed by equations of motion of the N bodies. Usually, integration of such a large system of equations is not feasible. Therefore we must use the statistical methods.

We first introduce the distribution function f_{pv}, which is defined by

$$\begin{aligned} &f_{pv}(\mathbf{r},\mathbf{v},t)\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v} \\ &\quad = (\text{the number of particles in the system that have} \\ &\qquad \text{phase points in } \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v} \text{ about } \mathbf{r} \text{ and } \mathbf{v} \text{ at time } t). \end{aligned} \tag{6}$$

Here $\mathbf{v}$ and $\mathbf{r}$ are with components v_i and r_i $(i = 1, 2, \ldots, l)$, respectively, $\mathrm{d}\mathbf{v} = \mathrm{d}v_1, \mathrm{d}v_2, \ldots, \mathrm{d}v_l$, and $\mathrm{d}\mathbf{r} = \mathrm{d}r_1, \mathrm{d}r_2, \ldots, \mathrm{d}r_l$. By this definition, we have

$$\int\int\int\cdots\int_{\text{all}\,\mathbf{r},\mathbf{v}} f_{pv}(\mathbf{r},\mathbf{v},t)\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v} = N. \tag{7}$$

The ensemble average of any function $\psi(\mathbf{r},\mathbf{v})$ of the position and velocity of the system is defined by

$$\langle\psi\rangle = \frac{1}{N}\int\int\int\cdots\int_{\text{all}\,\mathbf{r},\mathbf{v}} \psi(\mathbf{r},\mathbf{v},t) f_{pv}\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v}. \tag{8}$$

The assumption that the particles do not interact with each other leads to [2]

$$\frac{\mathrm{d}f_{pv}}{\mathrm{d}t} = 0. \tag{9}$$

This is called the *Liouville equation*. It indicates that if we follow the particles in a volume element along a flow line in phase space without collisions, the distribution is conserved,

$$f_{pv}(\mathbf{r}+\mathrm{d}\mathbf{r},\mathbf{v}+\mathrm{d}\mathbf{v},t+\mathrm{d}t) = f_{pv}(\mathbf{r},\mathbf{v},t). \tag{10}$$

If collisions occurs, the distribution f_{pv} will change over a time interval $\mathrm{d}t$ by an amount $(\partial f_{pv}/\partial t)_{\text{coll}}\mathrm{d}t$, and therefore

$$f_{pv}(\mathbf{r}+\mathrm{d}\mathbf{r},\mathbf{v}+\mathrm{d}\mathbf{v},t+\mathrm{d}t) - f_{pv}(\mathbf{r},\mathbf{v},t) = (\partial f_{pv}/\partial t)_{\text{coll}}\,\mathrm{d}t, \tag{11}$$

which is equivalent to

$$\frac{f_{pv}(\mathbf{r}+\mathrm{d}\mathbf{r},\mathbf{v}+\mathrm{d}\mathbf{v},t+\mathrm{d}t) - f_{pv}(\mathbf{r},\mathbf{v},t)}{\mathrm{d}t} = \left(\frac{\partial f_{pv}}{\partial t}\right)_{\text{coll}}. \tag{12}$$

Making use of the Taylor expansion of $f_{pv}(\mathbf{r}+\mathrm{d}\mathbf{r}, v+\mathrm{d}\mathbf{v}, t+\mathrm{d}t)$ at the point $(\mathbf{r},\mathbf{v},t)$, we have

$$\begin{aligned} &\frac{\sum_{j=1}^{l}\frac{\partial f_{pv}}{\partial r_j}\mathrm{d}r_j + \sum_{j=1}^{l}\frac{\partial f_{pv}}{\partial v_j}\mathrm{d}v_j + \frac{\partial f_{pv}}{\partial t}\mathrm{d}t + \text{higher order terms}}{\mathrm{d}t} \\ &\quad = \left(\frac{\partial f_{pv}}{\partial t}\right)_{\text{coll}}, \end{aligned} \tag{13}$$

equivalently,

$$\frac{\partial f_{pv}}{\partial t} + \sum_{j=1}^{l} v_j \frac{\partial f_{pv}}{\partial r_j} + \sum_{j=1}^{l} \frac{\partial v_j}{\partial t}\frac{\partial f_{pv}}{\partial v_j} = \left(\frac{\partial f_{pv}}{\partial t}\right)_{\text{coll}}. \tag{14}$$

This is the BTE. If we re-define the distribution function as

$$f(\mathbf{r},\mathbf{v},t) = \frac{f_{pv}(\mathbf{r},\mathbf{v},t)}{N},$$

then the BTE becomes

$$\frac{\partial f}{\partial t} + \sum_{j=1}^{l} v_j \frac{\partial f}{\partial r_j} + \sum_{j=1}^{l} \frac{\partial v_j}{\partial t}\frac{\partial f}{\partial v_j} = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}. \tag{15}$$

Usually, the collision term $\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$ in the BTE is handled by introducing a relaxation time, τ [2]

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{f - f_0}{\tau}, \tag{16}$$

with f_0 as the equilibrium distribution for the system. Suppose that a non-equilibrium distribution of velocities is set up by external forces which are suddenly removed.

The decay of the distribution towards equilibrium is then obtained from (16) as

$$\frac{\partial(f-f_0)}{\partial t}=-\frac{f-f_0}{\tau},$$

note that $\frac{\partial f_0}{\partial t}=0$ by definition of the equilibrium distribution. This equation has the solution

$$(f-f_0)|_t=(f-f_0)|_{t=0}\exp(-t/\tau).$$

Combining Eqs. (15) and (16), we obtain the BTE within the relaxation time approximation:

$$\frac{\partial f}{\partial t}+\sum_{j=1}^{l}v_j\frac{\partial f}{\partial r_j}+\sum_{j=1}^{l}\frac{\partial v_j}{\partial t}\frac{\partial f}{\partial v_j}=-\frac{f-f_0}{\tau}. \tag{17}$$

In the following, starting from Eqs. (12) and (16) not directly from Eq. (15), we try to re-establish the DPL model.

2.2. Derivation of DPL model

Consider a three-dimensional heat transfer problem. In this case, the position vector $\mathbf{r}$ has three components x, y and z, the velocity vector $\mathbf{v}$ is expressed as $(v_x,v_y,v_z)^{\mathrm{T}}$. To study the energy transport by particles, we must solve the BTE to determine the distribution function $f(\mathbf{r},\mathbf{v},t)$. In most cases, however, only an approximate distribution function can be obtained. If this distribution function is obtained, the rate of energy flow per unit area or the energy flux can then be expressed as

$$\mathbf{q}(\mathbf{r},t)=\int_{\text{all}\,\mathbf{v}}\mathbf{v}(\mathbf{r},t)f(\mathbf{r},\mathbf{v},t)\varepsilon(\mathbf{v})\,\mathrm{d}\mathbf{v}, \tag{18}$$

here $\mathbf{q}(\mathbf{r},t)$ is the energy flux vector, $\mathbf{v}(\mathbf{r},t)$ is the velocity vector, and $\varepsilon(\mathbf{v})$ is the kinetic energy of the particle as a function of particle velocity. Note that $f(\mathbf{r},\mathbf{v},t)$ is the fraction of system particles in the ensemble per unit volume per unit velocity. Therefore $f(\mathbf{r},\mathbf{v},t)\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v}$ is the fraction of system particles in the ensemble that have phase points in $\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v}$ about $\mathbf{r}$ and $\mathbf{v}$.

Equation (18) can be changed to an integral over momentum [18]:

$$\mathbf{q}(\mathbf{r},t)=\int_{\text{all}\,\mathbf{p}}\mathbf{v}(\mathbf{r},t)f(\mathbf{r},\mathbf{p},t)\varepsilon(\mathbf{p})\,\mathrm{d}\mathbf{p}, \tag{19}$$

where the vector $\mathbf{p}$ is the momentum and the distribution $f(\mathbf{r},\mathbf{p},t)$ is the fraction of system particles per unit volume per unit momentum. Therefore $f(\mathbf{r},\mathbf{p},t)\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{p}$ is the fraction of system particles in the ensemble that have phase points in $\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{p}$ about $\mathbf{r}$ and $\mathbf{p}$. Invoking the relation $\mathbf{p}=m\mathbf{v}$, we have

$$f(\mathbf{r},\mathbf{p},t)\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{p}=mf(\mathbf{r},\mathbf{p},t)\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v}. \tag{20}$$

This equation tells us that the fraction of system particles per unit volume and per unit velocity can also be expressed as $mf(\mathbf{r},\mathbf{p},t)$. Therefore we have the following relation:

$$f(\mathbf{r},\mathbf{v},t)=mf(\mathbf{r},\mathbf{p},t). \tag{21}$$

This equation enables us to rewrite Eq. (18) into Eq. (19).

Introducing the spherical coordinates for the integral in Eq. (19),

$$p_x=p\sin\theta\cos\varphi,\quad p_y=p\sin\theta\sin\varphi,\quad p_z=p\cos\theta,$$

where $p=\sqrt{p_x^2+p_y^2+p_z^2}$, we have

$$\mathbf{q}(\mathbf{r},t)=\int_0^\infty\int_0^\pi\int_0^{2\pi}\mathbf{v}(\mathbf{r},t)f(\mathbf{r},\mathbf{p},t)\varepsilon(\mathbf{p})p^2\sin\theta\,\mathrm{d}p\,\mathrm{d}\theta\,\mathrm{d}\varphi. \tag{22}$$

Invoking the relationship of p with the kinetic energy ε yields

$$\mathbf{q}(\mathbf{r},t)=\int_0^\infty\int_0^\pi\int_0^{2\pi}\mathbf{v}(\mathbf{r},t)f(\mathbf{r},\mathbf{p},t)\varepsilon m\sqrt{2m\varepsilon}\sin\theta\,\mathrm{d}\varepsilon\,\mathrm{d}\theta\,\mathrm{d}\varphi. \tag{23}$$

We assume that no external forces act on the heat transfer medium. Therefore the particle randomly accesses to every direction with the same probability. Under this assumption, we assert that the distribution function $f(\mathbf{r},\mathbf{p},t)$ only depends on the $\mathbf{r}$, ε and t. There is no bias on the directions of the momentum vector $\mathbf{p}$. In this circumstance, the density of states $D(\varepsilon)$ can be defined as

$$D(\varepsilon)=\int_0^\pi\int_0^{2\pi}m\sqrt{2m\varepsilon}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi=4\pi m\sqrt{2m\varepsilon}. \tag{24}$$

This is the classical definition of the density of states. If taking into account the quantum effect, for the electron, we have

$$D(\varepsilon)=\frac{m\sqrt{2m\varepsilon}}{\hbar^3\pi^2}, \tag{25}$$

where $\hbar$ is Planck's constant divided by 2π. By the density of states $D(\varepsilon)$, Eq. (23) can be further transformed to that over energy. Then the energy flux vector can be expressed as

$$\mathbf{q}(\mathbf{r},t)=\int_\varepsilon\mathbf{v}(\mathbf{r},t)f(\mathbf{r},\varepsilon,t)\varepsilon D(\varepsilon)\mathrm{d}\varepsilon. \tag{26}$$

From Eqs. (12) and (16), it follows that

$$\frac{f(\mathbf{r}+\mathrm{d}\mathbf{r},\varepsilon(\mathbf{v}+\mathrm{d}\mathbf{v}),t+\mathrm{d}t)-f(\mathbf{r},\varepsilon(\mathbf{v}),t)}{\mathrm{d}t}=\frac{f_0-f}{\tau}, \tag{27}$$

where $\mathrm{d}\mathbf{r}$ and $\mathrm{d}\mathbf{v}$ are the incremental of position and velocity vectors, respectively. Note that this equation is an approximation. To have the right side of Eq. (27),

$f(\mathbf{r},\varepsilon(\mathbf{v}),t)$ requires approximately τ periods of decay to the equilibrium state f_0. Under the assumption that no external forces act on the heat transfer medium, the acceleration is zero. Therefore Eq. (27) can be rewritten as

$$\frac{f(\mathbf{r}+\mathrm{d}\mathbf{r},\varepsilon(\mathbf{v}),t+\mathrm{d}t)-f(\mathbf{r},\varepsilon(\mathbf{v}),t+\mathrm{d}t)}{\mathrm{d}t} + \frac{f(\mathbf{r},\varepsilon(\mathbf{v}),t+\mathrm{d}t)-f(\mathbf{r},\varepsilon(\mathbf{v}),t)}{\mathrm{d}t} = \frac{f_0-f}{\tau}. \tag{28}$$

For the first term of Eq. (28), applying Taylor expansion of $f(\mathbf{r}+\mathrm{d}\mathbf{r},\varepsilon(\mathbf{v}),t+\mathrm{d}t)$ at the point $(\mathbf{r},\varepsilon(\mathbf{v}),t+\mathrm{d}t)$ gives

$$\frac{f(\mathbf{r}+\mathrm{d}\mathbf{r},\varepsilon(\mathbf{v}),t+\mathrm{d}t)-f(\mathbf{r},\varepsilon(\mathbf{v}),t+\mathrm{d}t)}{\mathrm{d}t} = \frac{\mathrm{d}\mathbf{r}\cdot\nabla f(\mathbf{r},\varepsilon(\mathbf{v}),t+\mathrm{d}t)+\text{higher order terms}}{\mathrm{d}t}. \tag{29}$$

Therefore, there exists a value τ_T such that the following expression:

$$\mathbf{v}\cdot\nabla f(\mathbf{r},\varepsilon(\mathbf{v}),t+\tau_T) \tag{30}$$

is the best approximation to the first term of Eq. (28). By assuming $\mathrm{d}t \approx \tau$ [18], Eq. (28) becomes

$$\tau\mathbf{v}\cdot\nabla f(\mathbf{r},\varepsilon(\mathbf{v}),t+\tau_T)+f(\mathbf{r},\varepsilon(\mathbf{v}),t+\tau)=f_0. \tag{31}$$

Multiplying $\varepsilon D(\varepsilon)\mathbf{v}$ on two sides of this equation and integrating over all possible energies yields

$$\int_\varepsilon \tau\mathbf{v}\cdot\nabla f(\mathbf{r},\varepsilon(\mathbf{v}),t+\tau_T)\mathbf{v}\varepsilon D(\varepsilon)\,\mathrm{d}\varepsilon+\mathbf{q}(\mathbf{r},\mathbf{v},t+\tau)=\mathbf{0}. \tag{32}$$

In deriving this equation, the relation

$$\int_\varepsilon f_0\varepsilon D(\varepsilon)\mathbf{v}\,\mathrm{d}\varepsilon=\mathbf{0} \tag{33}$$

has been used, which is verified in the following.

For the electron, f_0 is the Fermi–Dirac equilibrium distribution

$$f_0(\varepsilon)=\frac{1}{1+\exp\left(\frac{\varepsilon-\mu}{k_B T}\right)}, \tag{34}$$

where μ is the chemical potential, k_B the Boltzmann constant and T the temperature. For the phonon, f_0 is the Bose–Einstein equilibrium distribution

$$f_0(\varepsilon)=\frac{1}{\exp(\frac{\varepsilon}{k_B T})-1}, \tag{35}$$

where $\varepsilon=\hbar\omega$, ω is the angular frequency of the quantum harmonic oscillator. Obviously, in both cases, f_0 is an even function with respect to the velocity $\mathbf{v}$. Subsequently the integrand in Eq. (33) is an odd function with respect to the velocity $\mathbf{v}$. Therefore the integral in Eq. (33) vanishes.

Assume that the relaxation times τ_T and τ do not depend on the energy of the system and the system has achieved the quasi-equilibrium state. Then $\nabla f=(\mathrm{d}f_0/\mathrm{d}T)\nabla T$, and Eq. (32) becomes

$$\mathbf{q}(\mathbf{r},t+\tau)=-\mathbf{k}\cdot\nabla T(\mathbf{r},t+\tau_T), \tag{36}$$

where $\mathbf{k}$ is the thermal conductivity tensor,

$$\mathbf{k}=\int\tau\mathbf{v}\mathbf{v}\frac{\mathrm{d}f_0}{\mathrm{d}T}\varepsilon D(\varepsilon)\mathrm{d}D(\varepsilon).$$

For the isotropic materials, $\mathbf{k}$ takes the form of

$$\mathbf{k}=k\mathbf{I}.$$

Here $\mathbf{I}$ is the unit matrix and k is a constant. Eq. (36) reduces to

$$\mathbf{q}(\mathbf{r},t+\tau_q)=-k\nabla T(\mathbf{r},t+\tau_T), \tag{37}$$

where $\tau_q=\tau$. This is nothing but the dual-phase-lagging model (4). If we assume that $\tau_T=0$, Eq. (37) reduces to

$$\mathbf{q}(\mathbf{r},t+\tau)=-k\nabla T(\mathbf{r},t), \tag{38}$$

which is the single-phase-lagging model (3).

The first-order approximation of Eq. (37) gives

$$q(\mathbf{r},t)+\tau\frac{\partial\mathbf{q}}{\partial t}(\mathbf{r},t)\cong -k\left\{\nabla T(\mathbf{r},t)+\tau_T\frac{\partial}{\partial t}[\nabla T(\mathbf{r},t)]\right\}, \tag{39}$$

which is the approximate DPL model.

3. Delay/advanced dual-phase-lagging heat conduction equation

In this section, the relation (37) is directly employed to establish the governing equation of microscale heat conduction. This leads to the delay/advanced DPL heat conduction equation. After the initial and boundary conditions are prescribed, the initial–boundary value problem of the delay/advanced DPL heat conduction is formulated. The method of separation of variables is then applied to solve such problems.

3.1. Initial–boundary value problem of delay/advanced DPL heat conduction

In the present subsection, we aim to establish the governing equation of the DPL heat conduction and prescribe the initial and boundary conditions based on the constitutive equation (37). To achieve this, the following energy equation is required:

$$-\nabla\cdot\mathbf{q}(\mathbf{r},t)+Q(\mathbf{r},t)=C_p\frac{\partial T(\mathbf{r},t)}{\partial t}, \tag{40}$$

with C_p being the volumetric heat capacity, Q the volumetric heat source.

For time instant $t+\tau_q$, Eq. (40) becomes

$$-\nabla\cdot\mathbf{q}(\mathbf{r},t+t_q)+Q(\mathbf{r},t+\tau_q)=C_p\frac{\partial T(\mathbf{r},t+\tau_q)}{\partial t}. \tag{41}$$

The divergence of Eq. (37) leads to

$$\nabla\cdot\mathbf{q}(\mathbf{r},t+\tau_q)=-k\Delta T(\mathbf{r},t+\tau_{\mathrm{T}}), \tag{42}$$

where Δ is Laplacian operator.

The substitution of Eq. (42) into Eq. (41) yields

$$\Delta T(\mathbf{r},t+\tau_{\mathrm{T}})+\frac{1}{k}Q(\mathbf{r},t+\tau_q)=\frac{1}{\alpha}\frac{\partial T(\mathbf{r},t+\tau_q)}{\partial t}, \tag{43}$$

where $\alpha=\frac{k}{C_p}$.

Equation (43) is the delay/advanced governing equation of DPL heat conduction based on the constitutive Eq. (37).

If $\tau_q-\tau_{\mathrm{T}}>0$, Eq. (43) becomes

$$\Delta T(\mathbf{r},t'-\tau)+\frac{1}{k}Q(\mathbf{r},t')=\frac{1}{\alpha}\frac{\partial T(\mathbf{r},t')}{\partial t'},\quad \text{for } t'>\tau_q, \tag{44}$$

in which

$$t'=t+\tau_q,\quad \tau=\tau_q-\tau_{\mathrm{T}}.$$

This is a delay partial differential equation. Hereafter it is termed as the delay DPL heat conduction equation.

If $\tau_q-\tau_{\mathrm{T}}<0$, we obtain

$$\Delta T(\mathbf{r},t')+\frac{1}{k}Q(\mathbf{r},t'-\tau)=\frac{1}{\alpha}\frac{\partial T(\mathbf{r},t'-\tau)}{\partial t'},\quad \text{for } t'>\tau_{\mathrm{T}}, \tag{45}$$

in which

$$t'=t+\tau_{\mathrm{T}},\quad \tau=\tau_{\mathrm{T}}-\tau_q.$$

This is an advanced partial differential equation, and hereafter we term it as the advanced DPL heat conduction equation.

Let R, $S_i,(i=1,2,\ldots,s)$ be the heat conduction region considered and the boundary surfaces of the region R, respectively. The boundary condition of Eq. (44) or Eq. (45) is generally written as

$$k_i\frac{\partial T(\mathbf{r},t')}{\partial n_i}+h_iT(\mathbf{r},t')=f_i(\mathbf{r},t'),\quad \text{on the boundary surface } S_i, \tag{46}$$

where constants k_i and h_i satisfy $k_i^2+h_i^2\neq 0$; $\mathbf{n}=(n_1,n_2,n_3)$ is the outward normal of surface S. The initial condition for Eq. (44) [9] is

$$T(\mathbf{r},t')=\phi(\mathbf{r},t),\ \text{in the region } R,\quad t'\in[\tau_{\mathrm{T}},\tau_q]. \tag{47}$$

By using the relation between t and t', we also have

$$T(\mathbf{r},t)=\phi(\mathbf{r},t),\ \text{in the region } R,\quad \text{for } t\in[-\tau,0]. \tag{48}$$

For Eq. (45), the following initial condition should be specified [9]:

$$T(\mathbf{r},t')=\psi(\mathbf{r},t'),\ \text{in the region } R,\quad t'\in[\tau_q,\tau_{\mathrm{T}}]. \tag{49}$$

By converting t' into t, we have

$$T(\mathbf{r},t)=\psi(\mathbf{r},t),\ \text{in the region } R,\quad t\in[-\tau,0]. \tag{50}$$

When the lagging time τ is very small, initial conditions (48) and (50) are equivalent to specify all the time derivatives of temperature field at the initial moment, that is

$$\begin{aligned}&T(\mathbf{r},t)|_{t=0}=T_0(\mathbf{r}),\\&\left.\frac{\partial T(\mathbf{r},t)}{\partial t}\right|_{t=0}=T_1(\mathbf{r}),\\&\left.\frac{\partial^2 T(\mathbf{r},t)}{\partial t^2}\right|_{t=0}=T_2(\mathbf{r}),\ldots,\left.\frac{\partial^n T(\mathbf{r},t)}{\partial t^n}\right|_{t=0}=T_n(\mathbf{r}),\ldots,\end{aligned} \tag{51}$$

where T_n $(n=0,1,2,\ldots)$ are given functions of the position vector $\mathbf{r}$. Note that the initial–boundary conditions (48) and (50) are quite different from those of DPL heat conduction problems using the approximate DPL model (39).

3.2. Solution of delay DPL heat conduction problem

In this section the method of separation of variables is employed to obtain the solution of the initial–boundary condition problem of the delay DPL heat conduction.

From Section 3.1, the delay DPL heat conduction problem is mathematically formulated as

$$\frac{1}{\alpha}\frac{\partial T(\mathbf{r},t')}{\partial t'}=\Delta T(\mathbf{r},t'-\tau),\ \text{in the region } R,\quad \text{for } t'>\tau_q, \tag{52}$$

$$k_i\frac{\partial T(\mathbf{r},t')}{\partial n_i}+h_iT(\mathbf{r},t')=0,\quad \text{on the boundary surface } S_i, \tag{53}$$

$$T(\mathbf{r},t')=\phi(\mathbf{r},t'),\quad t'\in[\tau_{\mathrm{T}},\tau_q], \tag{54}$$

where $i=1,2,\ldots,s$, $\tau_q>\tau_{\mathrm{T}}$, $\phi(\mathbf{r},t')$ is a continuous function in the interval $[\tau_{\mathrm{T}},\tau_q]$.

By the method of separation of variables, let

$$T(\mathbf{r},t')=X(\mathbf{r})\Gamma(t'). \tag{55}$$

Substitution of Eq. (55) into Eq. (52) yields

$$\frac{1}{\alpha}\frac{\Gamma'(t')}{\Gamma(t'-\tau)}=\frac{\Delta X(\mathbf{r})}{X(\mathbf{r})}, \tag{56}$$

where $\Gamma'(t')$ is the derivative of $\Gamma(t')$ with respect to the time variable t'. Therefore,

$$\Gamma'(t')=-\alpha\beta^2\Gamma(t'-\tau), \tag{57}$$

$$\Delta X(\mathbf{r})+\beta^2X(\mathbf{r})=0, \tag{58}$$

where β is a real number. Substituting Eq. (55) into Eq. (53) leads to

$$k_i\frac{\partial X(\mathbf{r})}{\partial n_i}+h_iX(\mathbf{r})=0. \tag{59}$$

Thus Eqs. (58) and (59) form an eigenvalue problem. Note that this problem has non-trivial solutions only for certain discrete values of β. Such discrete values and solutions are called eigenvalues and eigenfunctions, respectively. Let β_i $(i = 1, 2, \ldots)$ be the eigenvalues, $X_i(\mathbf{r})$ $(i = 1, 2, \ldots)$ the corresponding eigenfunctions. A function $F(\mathbf{r})$ can be expanded as a generalized Fourier series

$$F(\mathbf{r}) = \sum_{i=1}^{\infty} F_i X_i(\mathbf{r}), \tag{60}$$

where

$$F_i = \frac{\int_R F(\mathbf{r}) X_i(\mathbf{r}) \mathrm{d}R}{\int_R X_i^2(\mathbf{r}) \mathrm{d}R}.$$

Substituting $\beta = \beta_i$ into Eq. (57) yields

$$\Gamma_i'(t') = -\alpha\beta_i^2 \Gamma_i(t' - \tau). \tag{61}$$

Assuming that we have found the solution of Eq. (61), the complete solution of the problem (52)–(54) can be written, by the superposition principle, as

$$T(\mathbf{r}, t') = \sum_{i=1}^{\infty} \Gamma_i(t') X_i(\mathbf{r}). \tag{62}$$

By applying the initial condition (54), we have

$$\sum_{i=1}^{\infty} \Gamma_i(t') X_i(\mathbf{r}) = \phi(\mathbf{r}, t'), \quad t' \in [\tau_{\mathrm{T}}, \tau_q],$$

which yields, by using the orthogonality of the eigenfunction set of $X_i(\mathbf{r})$,

$$\Gamma_i(t') = \phi_i(t'), \quad t' \in [\tau_{\mathrm{T}}, \tau_q]. \tag{63}$$

Here

$$\phi_i(t') = \frac{\int_R \phi(\mathbf{r}, t') X_i(\mathbf{r}) \mathrm{d}R}{\int_R X_i^2(\mathbf{r}) \mathrm{d}R} \quad (i = 1, 2, \ldots).$$

Note that Eqs. (61) and (63) constitute a problem of delay ordinary differential equations. We can use the method of steps or so called continuous method to solve this problem.

Integrating both sides of Eq. (61) over the interval $[\tau_q, t']$ yields

$$\Gamma_i(t') = \Gamma_i(\tau_q) - \alpha\beta_i^2 \int_{\tau_q}^{t'} \Gamma_i(t' - \tau) \mathrm{d}t'. \tag{64}$$

Note that if $t' \in [\tau_q, \tau_q + \tau]$,

$$\tau_{\mathrm{T}} \leqslant t' - \tau \leqslant \tau_q.$$

By Eq. (63), we thus have

$$\Gamma_i(t') = \phi_i(\tau_q) - \alpha\beta_i^2 \int_{\tau_q}^{t'} \phi_i(t' - \tau) \mathrm{d}t'. \tag{65}$$

We can proceed in this way by extending the definition of $\Gamma(t')$ from one interval to the next. Finally the solution of Eq. (61) subject to the initial condition (63) can be obtained.

3.3. Solution of advanced DPL heat conduction problem

In the present subsection, the method of separation of variables is applied to solve the advanced DPL heat conduction problem, which is mathematically formulated as follows, by Section 3.1,

$$\Delta T(\mathbf{r}, t') = \frac{1}{\alpha} \frac{\partial T(\mathbf{r}, t' - \tau)}{\partial t'}, \text{ in the region } R, \quad t' > \tau_{\mathrm{T}}. \tag{66}$$

$$k_i \frac{\partial T(\mathbf{r}, t')}{\partial n_i} + h_i T(\mathbf{r}, \quad t') = 0, \quad \text{on the boundary surface } S_i, \tag{67}$$

$$T(\mathbf{r}, t') = \psi(\mathbf{r}, t'), \quad t' \in [\tau_q, \tau_{\mathrm{T}}], \tag{68}$$

where $i = 1, 2, \ldots, s$, $k_i^2 + h_i^2 \neq 0$, $\psi(\mathbf{r}, t')$ has infinitely continuous derivatives with respect to the time variable t'.

By the method of separated variables

$$T(\mathbf{r}, t') = X(\mathbf{r}) \Gamma(t'). \tag{69}$$

Substituting Eq. (69) into Eq. (66) leads to

$$\frac{\frac{\partial \Gamma'(t'-\tau)}{\partial t'}}{\alpha \Gamma(t')} = \frac{\Delta X(\mathbf{r})}{X(\mathbf{r})}. \tag{70}$$

The condition under which Eq. (70) holds is that both sides of Eq. (70) is equal to a constant, say, $-\beta^2$,

$$\Delta X(\mathbf{r}) + \beta^2 X(\mathbf{r}) = 0, \tag{71}$$

$$\frac{\partial \Gamma'(t' - \tau)}{\partial t'} = -\alpha\beta^2 \Gamma(t'). \tag{72}$$

Substitution of Eq. (69) into Eq. (67) yields

$$k_i \frac{\partial X(\mathbf{r})}{\partial n_i} + h_i X(\mathbf{r}) = 0,$$

$$\text{on the boundary surfaces } S_i \quad (i = 1, 2, \ldots, s). \tag{73}$$

Hence Eqs. (71) and (73) constitute an eigenvalue problem. Let β_i $(i = 1, 2, 3, \ldots)$ be the eigenvalues, $X_i(\mathbf{r})$ the corresponding eigenfunctions. According to the Sturm–Liouville theory, the eigenfunctions $X_i(\mathbf{r})$ $(i = 1, 2, \ldots)$ have the orthogonal property.

Setting $\beta = \beta_i$ in Eq. (72) yields

$$\Gamma_i'(t' - \tau) = -\alpha\beta_i^2 \Gamma_i(t'). \tag{74}$$

If the solution of Eq. (74) is obtainable, the complete solution of the problem (66)–(68) can be written, by the superposition principle, as

$$T(\mathbf{r}, t') = \sum_{i=1}^{\infty} \Gamma_i(t') X_i(\mathbf{r}). \tag{75}$$

Substituting Eq. (75) into Eq. (68) yields

$$\sum_{i=1}^{\infty} \Gamma_i(t') X_i(\mathbf{r}) = \psi(\mathbf{r}, t'), \quad t' \in [\tau_q, \tau_{\mathrm{T}}], \tag{76}$$

which leads to, by the orthogonality of the set of functions $X_i(\mathbf{r})$,

$$\Gamma_i(t') = \psi_i(t'), \quad t' \in [\tau_q, \tau_T]. \tag{77}$$

Here

$$\psi_i(t') = \frac{\int_R \psi(\mathbf{r}, t') X_i(\mathbf{r}) \mathrm{d}R}{\int_R X_i^2(\mathbf{r}) \mathrm{d}R}.$$

Thus Eqs. (74) and (77) constitute a problem of advanced ordinary differential equation, which can be solved by the method of steps.

If $t' \in [\tau_T, \tau_T + \tau]$, it follows from Eqs. (74) and (77) that

$$\Gamma_i(t') = -\frac{1}{\alpha\beta_i^2} \frac{\partial \psi_i(t' - \tau)}{\partial t'}. \tag{78}$$

If $t' \in [\tau_T + \tau, \tau_T + 2\tau]$, we obtain from Eqs. (74) and (78)

$$\Gamma_i(t') = \frac{1}{\alpha^2\beta_i^4} \frac{\partial^2 \psi_i(t' - 2\tau)}{\partial t'^2}. \tag{79}$$

By continuing this process, $\Gamma_i(t')$ can be determined for every time instance t'.

4. Oscillation of delay/advanced DPL heat conduction

We know that the DPL heat conduction demonstrates wave-like behavior, such as the thermal oscillation and resonance [32]. It is interesting to examine whether the delay/advanced DPL heat conduction also exhibits the wave-like behavior.

First we present a fundamental result regarding the oscillation behavior of the delay/advanced ordinary differential equation [9].

Lemma 1. *Consider the differential equation*

$$\dot{\Gamma}(t) + p\Gamma(t - \tau) = 0, \tag{80}$$

where p and τ are two real numbers. Every solution of Eq. (80) oscillates if and only if

$$p\tau > \frac{1}{e}, \tag{81}$$

where $e = 2.71828\ldots$

Firstly, we attempt to seek the necessary and sufficient condition for the occurrence of oscillations of the delay differential equation

$$\dot{\Gamma}_i(t') = -\alpha\beta_i^2 \Gamma_i(t' - \tau), \quad t' > \tau_q, \tag{82}$$

where $\tau = \tau_q - \tau_T > 0$.

Applying Lemma 1 to Eq. (82), we readily obtain the following theorem.

Theorem 11.1. *The necessary and sufficient condition for every solution of Eq. (82) (it is a special case of (80) with $p = \alpha\beta_i^2$) to be oscillating is*

$$\alpha\beta_i^2\tau > \frac{1}{e} \quad (i = 1, 2, 3, \ldots). \tag{83}$$

Since the oscillation is a wave feature, the delay DPL heat conduction equation will have wave-like solution under the condition (83). Therefore the resonance could occur sometimes for the system with a temporally periodic heat source.

For the advanced differential equation, we have

$$\dot{\Gamma}_i(t - \tau) = -\alpha\beta_i^2 \Gamma_i(t), \quad t > \tau_T, \tag{84}$$

where $\tau = \tau_T - \tau_q$ is a non-negative constant. If we let

$$t' = t - \tau,$$

Eq. (84) becomes

$$\dot{\Gamma}_i(t') = -\alpha\beta_i^2 \Gamma_i(t' + \tau), \quad t' > \tau_q, \tag{85}$$

which is also a special case of Eq. (80) with τ replaced by $-\tau$ and $p = \alpha\beta_i^2$. However, because $\tau > 0$,

$$\alpha\beta_i^2(-\tau) < \frac{1}{e}. \tag{86}$$

Therefore, the solution of Eq. (84) will not oscillate by Lemma 1.

5. Concluding remarks

We assume that no external forces act on the heat transfer medium, the relaxation times τ_T and τ_q are independent on the energy of the system and the system has achieved the local quasi-equilibrium state. Under these assumptions, the dual-phase-lagging model is derived from the Boltzmann transport equation. This forms the foundation of the model. This model leads to a delay/advanced partial differential equation of microscale heat conduction. The initial–boundary problem of the delay/advanced partial differential equation is formulated mathematically. The method of separation of variables is applicable for solving this problem. The condition under which the thermal oscillation occurs is also established.

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