

Chapter 2

Dynamical Governing Equations of Non-Fourier Heat Conduction

Abstract Thermal energy has its corresponding equivalent mass according to Einstein's mass–energy equivalence, which is termed as thermomass. The thermomass theory established the continuous governing equation for the non-Fourier heat conduction. The mass balance equation of thermomass gives the energy conservation equation while the momentum balance equation of thermomass gives the general heat conduction law. The microscopic foundation of the general heat conduction law based on the thermomass theory is investigated. The derivation based on the phonon Boltzmann equation shows that the second order expansion of phonon distribution function leads to the spatial inertia (or convective) term in the general heat conduction law, which makes the difference from the previous phonon hydrodynamic model. Limiting to the first order expansion will give the Cattaneo-Vernotte model, while the zeroth order expansion gives the classical Fourier's law. Comparison with other derivations of phonon Boltzmann equation such as the Chapman–Enskog expansion and eigenvalue analysis is presented.

2.1 Mass–Energy Duality of Heat

In history, the nature of heat is regarded as either a fluid (caloric theory) or a type of motion (dynamic theory, kinetic theory, or mechanical theory). The caloric theory regards heat as a weightless, self-repulsive fluid. In the eighteenth and the first half of nineteenth centuries, the caloric theory was the mainstream theory. It gave explanations to the temperature change and phase change, and even contributed to the establishment of the Fourier's heat conduction law and the Carnot's rule for thermal engines. However, in the nineteenth century, a series of experiments showed the conversion between heat and work, such as Rumford's report of boring a cannon and Joule's measurement of the mechanical equivalent of heat. After the mid-nineteenth century, the caloric theory was generally superseded by the mechanical theory along with the acceptance of energy conservation law and kinetic theory of gas. The modern thermodynamic and heat transport theory is

based on the understanding that heat originates from the individually random, or disordered, motion of particles in a body.

In the twentieth century, Einstein's relativity theory introduced the well-known mass–energy equivalence relation, $E = mc^2$, where c is the speed of light. Therefore, all forms of energy correspond to a certain amount of mass. Consider a system consisting of n free particles, each having a mass m and a velocity v_i ; the rest mass of this system based on the relativity theory is

$$m_{0,\text{sys}} = \sum_{i=1}^n \frac{E_i}{c^2} \approx \sum_{i=1}^n \frac{m_{0,i}c^2 + (1/2)m_{0,i}v_i^2}{c^2} + o(v_i^2/c^2) \quad \text{with} \quad \sum_i m_{0,i}v_i = 0, \quad (2.1)$$

where m_0 is the rest mass of each particle. Equation 2.1 denotes that the rest mass of the system contains the total kinetic energy of individual particles, divided by c^2 . Heating the system increases the energy of the disordered motion of particles while the system's net momentum preserves zero. The increased rest mass due to heating has the same nature as ordinary mass, like inertia. Thus, greater force is needed to propel a heated body with the same acceleration than when it is cool [1–4]. According to the general relativity, the inertia mass equals the gravitational mass. Thus “a piece of iron weighs more when red-hot than when cool” [5, 6]. The mass increase induced by heat, “thermomass,” is very small in ordinary conditions. For example, the thermomass of Si at room temperature is 10^{-12} of the total mass. Such small amount of mass is negligible when dealing with dynamic problems such as movement and balance of the body. However, heat conduction is the movement of thermomass itself relative to the molecular or the lattice; so its mass, or inertia, should be accounted to describe the transport and motion of heat.

Moller [1] and Rindler et al. [4] analyzed the continuum mechanics in the relativity framework. The momentum flux for the relativity system with heat flux inside is expressed as

$$\mathbf{g} = \frac{h\mathbf{v} + \mathbf{v} \cdot \mathbf{\Pi} + \mathbf{J}}{c^2}, \quad (2.2)$$

where h is the relative energy density, \mathbf{v} is the velocity of the body, $\mathbf{\Pi}$ is the relative stress tensor, and \mathbf{J} is the energy flux density induced by heat conduction

$$\mathbf{J} = \gamma \left(\mathbf{q}^0 - \mathbf{v} \frac{\mathbf{q}^0 \cdot \mathbf{v}}{c^2} \frac{\gamma}{\gamma + 1} \right), \quad (2.3)$$

where γ is the Lorentz factor, $\gamma = (1 - v^2/c^2)^{-1/2}$. \mathbf{q}^0 is the heat flux density in the rest reference framework. In low speed systems where v is much less than c , the difference between \mathbf{J} and \mathbf{q} is the small amount of the order of $(v/c)^2$. In this case Eq. 2.2 can be converted into

$$\mathbf{g}^0 = (\rho^0 + \rho_E^0)\mathbf{v}^0 + \frac{\mathbf{v}^0 \cdot \boldsymbol{\Pi}^0}{c^2} + \frac{\mathbf{q}^0}{c^2}, \quad (2.4)$$

where the superscript 0 means the value in low speed system, ρ^0 is the density of rest mass of the molecular contained in the system, ρ_E^0 is the density of the equivalent mass of the energy (e.g., elastic energy, chemical energy, thermal energy, and nuclear bonding energy) stored in the system, divided by c^2 . Equation 2.4 shows that the momentum flux density of low speed system contains the momentum density of the rest mass (the first term on the right-hand side) plus the energy flux density divided by c^2 (the second and third terms on the right-hand side, which correspond to the work done by the stress and the heat flux, respectively). Note that the rest mass of the system contains the part contributed by the energy, $\rho_E^0 \mathbf{v}^0$. In normal conditions, the contribution by the heat flux is far more less than the first term. Nevertheless, consider a body at rest with heat conduction inside, i.e., $\mathbf{v}^0 = 0$, the heat flux term is the only nonzero one in Eq. 2.4.

Based on Eq. 2.4, in low speed conditions, the balance equation of mass and momentum can be expressed as

$$\frac{d}{dt^0}(\rho^0 + \rho_E^0) + \nabla \cdot \mathbf{g}^0 = 0 \quad (2.5)$$

$$\frac{d}{dt^0}\mathbf{g}^0 + \nabla \cdot \boldsymbol{\Pi}^0 + \frac{\mathbf{q}^0 \cdot \nabla \mathbf{v}^0}{c^2} = 0 \quad (2.6)$$

Using the mass conservation relation

$$\frac{d}{dt^0}\rho^0 + \nabla \cdot (\rho^0 \mathbf{v}^0) = 0 \quad (2.7)$$

Equation 2.5 turns to

$$\frac{d}{dt^0}\rho_E^0 + \nabla \cdot \left[\rho_E^0 \mathbf{v}^0 + \frac{\mathbf{v}^0 \cdot \boldsymbol{\Pi}^0}{c^2} + \frac{\mathbf{q}^0}{c^2} \right] = 0 \quad (2.8)$$

If the velocity of the body is zero, then Eq. 2.8 reduces to the energy balance equation (cf. Eq. 1.2). If the velocity is nonzero, then Eq. 2.8 is actually the energy balance equation in convective conditions. Equation 2.6 is equivalent to the Navier–Stokes equation without the body forces if the third term is neglected. On the other hand, for a rest body with heat conduction, $\mathbf{v}^0 = 0$, $\mathbf{q}^0 \neq 0$, the nonzero terms in Eq. 2.6 indicates that the heat flux is also driven by a stress tensor, as the momentum flux of rest mass. Note that Eq. 2.6 is built in the low speed system, thus the motion of \mathbf{q}^0 obeys Newton’s law of motion. In this way, for the heat flux in a rest body one has

$$\frac{d}{dt^0} \frac{\mathbf{q}^0}{c^2} = -\nabla \cdot \boldsymbol{\Pi}^0 \quad (2.9)$$

In ordinary conditions, the stress tensor, $\boldsymbol{\Pi}^0$, acting on the heat flux is very small. However, the quantity of thermomass is also very small, so the thermomass can be driven by the stress tensor with a recognizable acceleration.

Based on the above discussion, the thermomass, although derived from the relativity theory, obeys Newton's law of motion as long as it is discussed in low speed systems. Therefore, the dynamical governing equation of the motion of thermomass can be established to analyze the heat conduction processes from the ab initio viewpoint.

2.2 Governing Equations of Phonon Gas Dynamics

Phonons are the main heat carriers of dielectric solids, which come from the quantization of the lattice vibration. The heat conduction in dielectric solids is thus determined by the transport of phonons. In the thermal equilibrium system, the distribution function of phonons, f , satisfies the Bose–Einstein distribution, namely obeys the Planck's law [7, 8]

$$f_0 = [\exp(\hbar\omega/k_B T) - 1]^{-1}, \quad (2.10)$$

where \hbar is the reduced Planck constant (Dirac constant), ω is the phonon frequency, and k_B is the Boltzmann constant. The collective behavior of phonons is like a gas, namely phonon gas. The energy carried by the phonon gas in a unit volume is

$$\begin{aligned} e &= \rho C_V T = (2\pi)^{-3} \sum_n \int [\hbar\omega^n f^n(\mathbf{k}, \mathbf{x}, t)] d^3k \\ &= \sum_n \int_k \hbar\omega^n f^n(\mathbf{k}, \mathbf{x}, t) \end{aligned} \quad (2.11)$$

where i is the number of phonon branches, k is the wave vector. Inserting Eq. 2.11 into Eq. 2.1 gives

$$m_{0,\text{sys}} = \frac{\sum_i m_{0,i} c^2 + \sum_n \int_k \hbar\omega^n f^n dk}{c^2} + o\left(\sum_n \int_k \hbar\omega^n f^n dk / c^2\right) \quad (2.12)$$

Thus the density of the equivalent mass of phonon gas can be defined as

$$\rho_h = \frac{\rho C_V T}{c^2} \quad (2.13)$$

The motion of phonon gas is regarded as a weighable fluid flowing diffusively through a porous medium (the framework of lattice). The drift velocity is the mass flux q/c^2 dividide by the density ρ_h

$$\mathbf{u}_h = \frac{\mathbf{q}}{\rho C_V T} \quad (2.14)$$

With the definition of mass and velocity, one can establish the mass and momentum balance equations of the phonon gas

$$\frac{\partial \rho_h}{\partial t} + \nabla \cdot (\rho_h \mathbf{u}_h) = 0 \quad (2.15)$$

$$\rho_h \frac{\partial \mathbf{u}_h}{\partial t} + (\rho_h \mathbf{u}_h \cdot \nabla) \mathbf{u}_h + \nabla p_h = \mathbf{f}_h, \quad (2.16)$$

where p_h is the phonon gas pressure, f_h is the friction force impeding the phonon gas. Inserting Eqs. 2.13 and 2.14 into Eq. 2.15 yields the energy balance equation for solids, Eq. 1.2. The momentum balance equation of phonon gas describes the heat transport in dielectric solids. Guo et al. derived the expression for the phonon gas pressure [9–13]

$$p_h = \gamma_G \rho_h C_V T = \frac{\gamma_G \rho (C_V T)^2}{c^2}, \quad (2.17)$$

where γ_G is the Grüneisen parameter. In bulk materials, the friction force acting on the phonon gas is proportional to its drift velocity, which is similar to the case of porous flow

$$\mathbf{f}_h = -\chi \rho_h \mathbf{u}_h \quad (2.18)$$

Equation 2.16 reduces to the Fourier's heat conduction law when the inertia effect is negligible. The friction factor in Eq. 2.18 can thereby be determined as

$$\chi = 2\gamma_G \rho C_V^2 T / \kappa \quad (2.19)$$

Substitution of Eqs. 2.18 and 2.19 into the momentum balance relation, Eq. 2.16, gives the general heat conduction law [9–13]

$$\tau_{TM} \frac{\partial \mathbf{q}}{\partial t} + 2(\mathbf{l} \cdot \nabla) \mathbf{q} - b\kappa \nabla T + \kappa \nabla T + \mathbf{q} = 0, \quad (2.20)$$

where

$$\tau_{\text{TM}} = \frac{\kappa}{2\gamma_{\text{G}}\rho C_V^2 T} \quad (2.21a)$$

$$l = \frac{q\kappa}{2\gamma_{\text{G}}C_V(\rho C_V T)^2} = u_{\text{h}}\tau_{\text{TM}} \quad (2.21b)$$

$$b = \frac{q^2}{2\gamma_{\text{G}}\rho^2 C_V^3 T^3} = Ma_{\text{h}}^2 \quad (2.21c)$$

τ_{TM} is the characteristic lagging time between the temperature gradient and the heat flux, which relates to the wave-like heat transport predicted by the relaxational models. The characteristic length l measures the spatial inertia of thermomass, which predicts the size effect in nanowires and nanotubes [14–16]. $v_{\text{s}} = (2\gamma_{\text{G}}C_V T)^{1/2}$ is the propagation speed of disturbance in phonon gas. The Mach number of phonon gas, $Ma_{\text{h}} = u_{\text{h}}/v_{\text{s}}$, represents the compressibility of phonon gas, which predicts the heat flow choking in CNTs [17]. The first term in Eq. 2.20 is the transient inertia. The second and third terms are the spatial inertia. The forth term is the driving force and the last term is the friction force. If all the inertia terms are neglected, one recovers the Fourier's heat conduction law, which is in analogy with the Darcy's law in porous flow. If only the spatial inertia term is negligible, one retrieves the Cattaneo-Vernotte (CV) model from Eq. 2.20.

Define the objective derivative as

$$D/Dt = \partial/\partial t + 2(u_{\text{h}} \cdot \nabla) \quad (2.22)$$

Thus Eq. 2.20 can be rewritten as

$$\tau_{\text{TM}} \frac{Dq}{Dt} + q = -\kappa(1-b)\nabla T \quad (2.23)$$

The main differences between the general heat conduction law based on the thermomass theory and CV model are: (1) The objective derivative D/Dt replaces the partial derivative, $\partial/\partial t$; (2) The driving term contains additional parameter $1-b$. The first difference arises from accounting for the convective effective of phonon gas, namely the spatial inertia. Christov and Jordan [18] indicated that in a moving medium, the objective derivative should be selected as $D/Dt = \partial/\partial t + v \cdot \nabla$, in order to avoid the paradox of breaking Galileo invariance during heat wave propagation. Note that v is the moving speed of the medium where heat conduction occurs, rather than the drift velocity of phonon gas. Usually the drift velocity of phonon gas is far less than the speed of conduction medium. However, in ultrasmall medium, l , namely the product of drift velocity and relaxation time, could be comparable with the characteristic size of system. In this case the convection effect of phonon gas needs to be considered. Müller and Ruggeri [19] proposed that the objective derivative in the case of heat conduction in gases should have the form $Dq_i/Dt = \partial q_i/\partial t + q_k(\partial u_i/\partial x_k) - 2q_k W_{ik}$, where W is the angular velocity matrix.

The second term, $q_k(\partial u_i/\partial x_k)$, arises from the requirement of “objectivity”, like the Jaumann derivative in the theory of non-Newtonian fluid. The third term can be written as $-2c^2(\rho_h u_h)_k W_{ik}$. It is actually the Coriolis effect induced by the rotation of conduction medium. The second difference relates to the definition of temperature during non-Fourier heat conduction, which will be discussed in detail in Chap. 4.

The derivation of Eq. 2.20 assumes the linear relation between friction and drift velocity. In the porous flow, when the flow region is near boundary, the Darcy’s law needs to be modified into Darcy–Brinkman law. Thus the friction contains both the linear term of velocity and the second spatial derivative of velocity, i.e.,

$$\mathbf{f}_h = -\chi \rho_h \mathbf{u}_h + \mu_h \nabla^2 \mathbf{u}_h \quad (2.24)$$

where μ_h is the viscosity of phonon gas. Substitution of Eq. 2.24 into the momentum balance equation of phonon gas, Eq. 2.16, one has

$$\tau_{\text{TM}} \frac{\partial \mathbf{q}}{\partial t} + 2l \nabla \mathbf{q} - b \kappa \nabla T + \kappa \nabla T + \mathbf{q} - l_B^2 \nabla^2 \mathbf{q} = 0, \quad (2.25)$$

where

$$l_B = \sqrt{\mu_h / \chi \rho_h} \quad (2.26)$$

The Brinkman term, $\mu_h \nabla^2 \mathbf{u}_h$, indicates a boundary layer where the boundary friction is important. The characteristic thickness of the boundary layer for the phonon gas is l_B . At room temperature, l_B usually has the value $10 \sim 100$ nm. Therefore, the Brinkman effect only needs to be considered in nanosystems.

Equation 2.25 has a form similar to the phonon hydrodynamic model, Eq. 1.7. The latter is obtained through the solution of the linear phonon Boltzmann equation. In the following section the phonon Boltzmann derivation of Eq. 2.25 is discussed.

2.3 Microscopic Foundation

2.3.1 Phonon Boltzmann Derivation

As long as the system size is much larger than the phonon wavelength (typically less than a few nanometers for dielectric materials at room temperature), the aggregate behavior of phonons can be characterized by the Boltzmann equation. The state distribution function, f , is desired to be solved from the Boltzmann equation so as to give the governing equations of macroscopic quantities such as temperature and heat flux. Many assumptions are made in solving the phonon Boltzmann equation, which thereby influence the results of solution. The derivation here will be combined with the recognition that the phonon gas is a weighable fluid, and compared with other solution methods of the phonon Boltzmann equation.

The phonon Boltzmann equation generally has the form [20, 21]

$$Df(\mathbf{k}, \mathbf{x}, t) = Cf(\mathbf{k}, \mathbf{x}, t) \quad (2.27)$$

where D and C are the drift and collision operator, respectively. The macroscopic variables, such as the internal energy density e and the heat flux density q , can be obtained by the integral of microscopic distribution function

$$e = \sum_n \int_k \hbar \omega^n f^n \quad (2.28)$$

$$q_i = \sum_n \int_k \hbar \omega^n \frac{\partial \omega^n}{\partial k_i} f^n \quad (2.29)$$

Guyer and Krumhansl [20, 21] obtained the eigenvalue solution of Eq. 2.27 which leads to the phonon hydrodynamics model, Eq. 1.7. Sussmann and Thellung [22] also obtained the governing equation similar to Eq. 1.7 by assuming that the Umklapp scattering rate is rare in pure crystals at low temperature. The Umklapp scattering and other phonon quasi-momentum ($\hbar k$) breaking scattering processes are called the resistive (R) processes. In contrast, the normal (N) scattering processes conserve the phonon quasi-momentum. The R processes incline to relax f to the equilibrium Planck distribution, i.e., f_0 in Eq. 2.10. The N processes incline to relax f to the displaced Planck distribution

$$f_D = \frac{1}{\exp[(\hbar \omega - \hbar \mathbf{k} \cdot \mathbf{u}_D)/k_B T] - 1}, \quad (2.30)$$

where u_D has the dimension of velocity. It is also called the drift velocity of phonon gas. The drift operator in Eq. 2.27 can be written as $D = \partial/\partial t + \mathbf{v}_k \cdot \nabla$, where \mathbf{v}_k is the group velocity of phonons

$$\mathbf{v}_k = \frac{\partial \omega}{\partial \mathbf{k}} \quad (2.31)$$

In this way, the phonon Boltzmann equation can be approximated by a relaxation form

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_k^n \cdot \nabla \right) f^n = \frac{f_0^n - f^n}{\tau_R} + \frac{f_D^n - f^n}{\tau_N} \quad (2.32)$$

In pure crystals at low temperature, the N processes overwhelm R processes. In this case $\tau_N \ll \tau_R$, the phonon distribution function is close to f_D . Approximating f with f_D can reveal the structure of the solution. In more general cases, the phonon distribution can be expressed as $f = f_D + f_N$, which is further deliberated in

Sect. 2.3.2. The actual relaxation time depends on the phonon frequency, branches, and temperature. For simplicity, the constant values of τ_R and τ_N are used for the present discussion.

Substitution of $f = f_D$ into Eq. 2.32 leads to

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_k^n \cdot \nabla \right) f_D^n = \frac{f_0^n - f_D^n}{\tau_R} \quad (2.33)$$

Integral of Eq. 2.33 in the k space with multiplying $\hbar k_i$ or $\hbar \omega_{v_{ki}}$ will give the macroscopic governing equations which predicts the drifting or driftless second sound, respectively [23, 24]. The difference between the two types of second sound can be shown as

$$\frac{v'_{II}}{v_{II}} = \frac{\sum_{\text{all } \varepsilon} \langle 0 | v^1 | \varepsilon \rangle \langle \varepsilon | v^1 | 0 \rangle}{\sum_{\varepsilon=0}^3 \langle 0 | v^1 | \varepsilon \rangle \langle \varepsilon | v^1 | 0 \rangle}, \quad (2.34)$$

where $\langle \alpha | v | \beta \rangle$ is the matrix element expressed by the eigenvalue, v_{II} and v'_{II} are the velocities of drifting and driftless second sound, respectively. Therefore, the integral path of the driftless second sound, namely multiplying with $\hbar \omega_{v_{ki}}$ covers more eigenvalues than that of the drift second sound. Hardy [23] indicated that "... such a possibility suggests that the different types of second sound should be thought of not as distinct 'modes' of heat propagation, but rather as simply different approximation schemes which lead to the same phenomena."

The second integral method is favorable according to the thermomass theory. In the gas transport theory, multiplying the Boltzmann equation with the molecular momentum, mv , and integrating in the velocity space will lead to the momentum balance equation of fluid. According to the mass energy equivalence, $\hbar \omega$ is the phonon energy and $\hbar \omega / c^2$ is the equivalent mass of phonons. $\hbar \omega_{v_{ki}} / c^2$ is the phonon momentum accompanied by the heat transport. It is an actual momentum rather than the quasi-momentum of phonons, $\hbar k$. Similar to the transport theory of gases, multiplying Eq. 2.33 with $\hbar \omega / c^2$ and $\hbar \omega_{v_{ki}} / c^2$ and making integral, respectively, will give the mass and momentum balance equation of phonon gas. The distinction from the ordinary gas flow is that the phonon gas is also impeded by the R processes, which is reflected by the additional sink term of momentum, namely the collision operator on the right-hand side of Eq. 2.33. It is equivalent to the gas flow in a pipe filled with porous medium rather than empty.

Multiplying Eq. 2.33 with $\hbar \omega / c^2$ or $\hbar \omega_{v_{ki}} / c^2$ and then integrating in the k space yields

$$\frac{\partial \int_k f_D^n \hbar \omega^n}{\partial t} + \int_k \mathbf{v}_k^n \cdot \nabla f_D^n \hbar \omega^n = \frac{\int_k (f_0^n - f_D^n) \hbar \omega^n}{\tau_R} \quad (2.35)$$

$$\frac{\partial \int_{\mathbf{k}} f_{\mathbf{D}}^n \hbar \omega^n v_{ki}^n}{\partial t} + \int_{\mathbf{k}} \mathbf{v}_{\mathbf{k}}^n \cdot \nabla f_{\mathbf{D}}^n \hbar \omega^n v_{ki}^n = \frac{\int_{\mathbf{k}} (f_0^n - f_{\mathbf{D}}^n) \hbar \omega^n v_{ki}^n}{\tau_{\mathbf{R}}} \quad (2.36)$$

In order to integrate Eqs. 2.35 and 2.36, the feature of $f_{\mathbf{D}}$ needs to be discussed. The derivative of $f_{\mathbf{D}}$ with respect to the drift velocity is

$$\frac{\partial f_{\mathbf{D}}}{\partial u_{\mathbf{D}j}} = \frac{\hbar k_j}{k_{\mathbf{B}} T} \frac{\exp[(\hbar \omega - \hbar \mathbf{k} \cdot \mathbf{u}_{\mathbf{D}})/k_{\mathbf{B}} T]}{\{\exp[(\hbar \omega - \hbar \mathbf{k} \cdot \mathbf{u}_{\mathbf{D}})/k_{\mathbf{B}} T] - 1\}^2}, \quad (2.37)$$

while the derivative of f_0 with respect to frequency is

$$\frac{\partial f_0}{\partial \omega} = \frac{\hbar}{k_{\mathbf{B}} T} \frac{\exp(\hbar \omega / k_{\mathbf{B}} T)}{[\exp(\hbar \omega / k_{\mathbf{B}} T) - 1]^2} \quad (2.38)$$

Therefore, when $u_{\mathbf{D}}$ is not large one can approximate that

$$\frac{\partial f_{\mathbf{D}}}{\partial u_{\mathbf{D}j}} \approx k_j \frac{\partial f_0}{\partial \omega} \quad (2.39)$$

In the same manner, the second order derivative of $f_{\mathbf{D}}$ with respect to $u_{\mathbf{D}}$ is

$$\begin{aligned} \frac{\partial^2 f_{\mathbf{D}}}{\partial u_{\mathbf{D}j}^2} &= \frac{\hbar k_j}{k_{\mathbf{B}} T} \frac{\partial}{\partial u_{\mathbf{D}j}} \frac{\exp[(\hbar \omega - \hbar \mathbf{k} \cdot \mathbf{u}_{\mathbf{D}})/k_{\mathbf{B}} T]}{\{\exp[(\hbar \omega - \hbar \mathbf{k} \cdot \mathbf{u}_{\mathbf{D}})/k_{\mathbf{B}} T] - 1\}^2} \\ &= \left(\frac{\hbar k_j}{k_{\mathbf{B}} T} \right)^2 \mathfrak{X} \left[\frac{1}{(\mathfrak{X} - 1)^2} - \frac{2\mathfrak{X}}{(\mathfrak{X} - 1)^3} \right], \\ &\approx k_j^2 \frac{\partial^2 f_0}{\partial \omega^2} \end{aligned} \quad (2.40)$$

where

$$\mathfrak{X} = \exp[(\hbar \omega - \hbar \mathbf{k} \cdot \mathbf{u}_{\mathbf{D}})/k_{\mathbf{B}} T] \quad (2.41)$$

With the above results one can make a second order Taylor expansion of $f_{\mathbf{D}}$ around f_0

$$\begin{aligned} f_{\mathbf{D}} &= f_0 + \left. \frac{\partial f_{\mathbf{D}}}{\partial \mathbf{u}_{\mathbf{D}}} \right|_{\Delta \mathbf{u}_{\mathbf{D}}=0} \Delta \mathbf{u}_{\mathbf{D}} + \frac{1}{2} \left. \frac{\partial^2 f_{\mathbf{D}}}{\partial \mathbf{u}_{\mathbf{D}}^2} \right|_{\Delta \mathbf{u}_{\mathbf{D}}=0} (\Delta \mathbf{u}_{\mathbf{D}})^2 + o((\Delta \mathbf{u}_{\mathbf{D}})^2) \\ &= f_0 + \frac{\partial f_0}{\partial \omega} (\mathbf{k} \cdot \mathbf{u}_{\mathbf{D}}) + \frac{1}{2} \frac{\partial^2 f_0}{\partial \omega^2} (\mathbf{k} \cdot \mathbf{u}_{\mathbf{D}})^2 + o((\Delta \mathbf{u}_{\mathbf{D}})^2) \\ &= f_0 + f_+ + f_{++} + o((\Delta \mathbf{u}_{\mathbf{D}})^2) \end{aligned} \quad (2.42)$$

Note that f_0 and f_{++} are both even functions in the k space, while f_+ is an odd function. Substitution of Eq. 2.42 into Eqs. 2.35 and 2.36 gives

$$\frac{\partial \int_{\mathbf{k}} (f_0^n + f_{++}^n) \hbar \omega^n}{\partial t} + \nabla_j \int_{\mathbf{k}} f_+^n \hbar \omega^n v_{kj}^n = - \frac{\int_{\mathbf{k}} f_{++}^n \hbar \omega^n}{\tau_R} \quad (2.43)$$

$$\frac{\partial \int_{\mathbf{k}} f_+^n \hbar \omega^n v_{ki}^n}{\partial t} + \nabla_j \int_{\mathbf{k}} (f_0^n + f_{++}^n) \hbar \omega^n v_{ki}^n v_{kj}^n = - \frac{\int_{\mathbf{k}} f_+^n \hbar \omega^n v_{ki}^n}{\tau_R} \quad (2.44)$$

The second term on the left-hand side of Eq. 2.43 can be detailed as

$$\int_{\mathbf{k}} f_+^n \hbar \omega^n v_{kj}^n = \frac{4}{3} u_{Dj} \int_{\mathbf{k}} f_0^n \hbar \omega^n = \frac{4}{3} u_{Dj} e = q_j \quad (2.45)$$

The second order term, f_{++} , should be much smaller than f_0 , so its contribution to the internal energy is temporally neglected here. Further discussion is made in Sect. 4.4.

Note that u_D has a dimension of velocity, which relates to the drift velocity of thermomass as

$$u_D = \frac{3}{4} u_h \quad (2.46)$$

This velocity is called the average drift velocity of phonon gas [25]. However, without defining the mass of phonon gas, the physics of this velocity is ambiguous. Similarly, the velocity

$$u'_D = \frac{3q}{\rho C_V T} = 3u_h \quad (2.47)$$

is defined as the “fluid velocity” of phonon gas by Guyer and Krumahansl [20, 21]. It is also proportional to the drift velocity of thermomass. The difference between u'_D and u_h comes from the average of the homogeneous vector space.

Since the energy conservation is ensured during phonon scatterings, $\hbar \omega$ is the eigenvector of the zero space of the scattering operator, as well as the integral invariance of the Boltzmann equation. Therefore, Eq. 2.43 transforms to

$$\frac{\partial e}{\partial t} + \nabla_j q_j = 0 \quad (2.48)$$

which yields the traditional energy conservation equation. Integral of the second term on the left-hand side of Eq. 2.44 can be divided into an equilibrium and a nonequilibrium part

$$\int_k (f_0^n + f_{++}^n) \hbar \omega^n v_{ki}^n v_{kj}^n = \delta_{ij} \int_k f_0^n \hbar \omega^n v_{ki}^n v_{kj}^n + \int_k f_{++}^n \hbar \omega^n v_{ki}^n v_{kj}^n \quad (2.49)$$

Integration by parts of the second term on the right-hand side of Eq. 2.49 gives

$$\int_k f_{++}^n \hbar \omega^n v_{ki}^n v_{kj}^n = \frac{5}{3} u_{Di} u_{Dj} e \quad (2.50)$$

Inserting Eqs. 2.45, 2.49 and 2.50 into Eq. 2.44 leads to

$$\frac{\partial q_i}{\partial t} + \frac{15}{16} \nabla_j \frac{q_i q_j}{e} + \frac{1}{3} \nabla_j \int_k f_0^n \hbar \omega^n (v_k^n)^2 = -\frac{q_i}{\tau_R} \quad (2.51)$$

where the cubic symmetry is assumed to obtain the third term on the left-hand side of Eq. 2.51.

Equation 2.51 is actually the momentum balance equation of phonon gas. Compared with Eq. 2.20, which can be reformed as

$$\frac{\partial q_i}{\partial t} + \nabla_j \frac{q_i q_j}{e} + \nabla_i p_h = -\chi \frac{q_i}{e} \quad (2.52)$$

one observes that the homogeneous phonon gas pressure and be expressed by the integration of the microscopic phonon properties

$$p_h = \frac{1}{3} \int_k f_0^n \frac{\hbar \omega^n}{c^2} (v_k^n)^2 = \iiint_{\pm\pi/a} f_0^n(\mathbf{x}, t, \mathbf{k}) \frac{\hbar \omega^n}{c^2} (v_{kx}^n)^2 dk_x dk_y dk_z \quad (2.53)$$

It is notable that the gas pressure in the kinetic theory is expressed by

$$p_x = \iiint_{\pm\infty} f(\mathbf{x}, t, \mathbf{v}) m v_x^2 dv_x dv_y dv_z, \quad (2.54)$$

where p is the thermodynamic pressure, f is the local distribution function, m is the molecular mass, and \mathbf{v} is the velocity of each molecule. The integral structure of Eq. 2.54 is similar to that of Eq. 2.53. Thus the temperature gradient driving the heat flux has the similar physical meaning to the pressure gradient driving the gas flow.

The thermomass pressure is macroscopically derived from the Debye state equation of dielectric solids. According to the concept of thermomass, the phonons have the real momentum, $\hbar \omega v_{ki}/c^2$. In equilibrium state, the phonons are confined in the medium. Assume that the phonons are reflected at the boundary, i.e., the wave vector is reversed, the pressure of phonons can be calculated in analogy with the

ideal gas model. The impulse on the boundary is obtained through the momentum change of phonons. The characteristic velocity of phonons is defined as

$$v_g^2 = \frac{\sum_n \frac{1}{3} \int_k f_0^n \frac{\hbar \omega_k^n}{c^2} (v_k^n)^2}{\sum_n \int_k f_0^n \frac{\hbar \omega_k^n}{c^2}} \quad (2.55)$$

The denominator of Eq. 2.55 is the density of the equivalent mass of phonon gas, ρ_h . The relation between the phonon gas pressure and phonon gas density is

$$p_h = \frac{v_g^2}{c^2} \rho C_V T = v_g^2 \rho_h \quad (2.56)$$

Comparison with phonon gas pressure given by the thermomass theory yields

$$v_g = \sqrt{\gamma_G C_V T} \quad (2.57)$$

Thus v_g is not a constant but depends on the temperature. Also, v_g is different from the propagation speed of disturbance of phonon gas, v_s , which has the form

$$v_s = \sqrt{\frac{dp_h}{d\rho_h}} = \sqrt{2\gamma_G C_V T} \quad (2.58)$$

Equation 2.58 is in analogy with the relation between the density, pressure, and sound speed of ideal gas. The difference between v_s and v_g arises from the compression ratio of phonon gas (thermomass fluid). The propagation of small disturbance in ideal gas is well approximated by the adiabatic thermodynamic process. The compression ratio for the sound speed is determined by the density-pressure relation in an adiabatic process. The density and pressure of phonon gas satisfy

$$p_h \rho_h^{-2} = \text{const} \quad (2.59)$$

Thus the defaulted compression ratio of phonon gas is 2. Since the thermomass density directly depends on the pressure, there is no difference between the isothermal and adiabatic processes. In a non-dispersive medium, assuming that there is only one longitudinal phonon branch (L) and two translational branches (T), with the sound speed v_L and v_T , respectively, one has [23, 24]

$$v_g^2 = \frac{1}{3} \frac{v_L^{-1} + 2v_T^{-1}}{v_L^{-3} + 2v_T^{-3}} \quad (2.60)$$

Thus v_g is a weighted average of the sound speed of each phonon branch. If there is no coupling among phonon branches, the disturbance in each branch will propagate separately, causing a rapid dispersion of temperature wave. In this case there is no steady “temperature wave,” in other words, the heat wave will not form in such

medium. On the other hand, if the phonon can change branches frequently by scattering, namely the phonon in the L branch can transform into phonons in T branches and vice versa, a steady wave propagating with an average sound speed could form in medium. The former situation is close to the case in pure crystals at low temperature. The dispersion of temperature wave is also observable in MD simulations. At higher temperatures, the scattering among high frequency phonons rapidly redistributes the energy and momentum of phonon branches. In this case, the collective behavior of phonons is more likely a gas, which is describable by a continuous model. Equation 2.60 is actually the speed of the driftless second sound proposed by Hardy [23, 24], v'_{II} . For the drift second sound, the speed is

$$v_{II} = \frac{1}{3} \frac{v_L^{-3} + 2v_T^{-3}}{v_L^{-5} + 2v_T^{-5}} \quad (2.61)$$

The difference between v_{II} and v'_{II} originates from the multipliers used in integration, which are $\hbar k$ and $\hbar \omega v_{ki}/c^2$, respectively. It induces different weight for the sound speeds of phonon branches. Enz [26] pointed out that distinction of the driftless second sound from the drift one is decided by the fact of whether the core variable during second sound propagation is the quasi-momentum or energy flux (heat flux). It can be inferred that the drift second sound is more likely to happen in the pure crystal at low temperature. However, the dispersion is strong for heat waves. It can only maintain a stable wave within a short propagation distance. For medium at higher temperatures, the driftless second sound is possible. In this case, dissipation during heat wave propagation is strong. The heat wave is easily merged in the noise caused by R scatterings. If a medium can satisfy the conditions of large MFP for R processes and small N processes, the differences among sound speeds of different phonon branches are small or the propagation is dominated by one phonon branch while other branches contribute little to the heat transfer, the heat wave is more likely to be observable. It is expected that low-dimensional material (such as CNT and graphene) could be good candidates for measuring the heat wave.

Equation 2.51 indicates that the phonon gas pressure plays the role of driving force of heat conduction. For a specific material, the phonon gas pressure can be obtained either from the macroscopic approach, i.e., Eq. 2.17, or the microscopic expression, Eq. 2.53. The phonon gas pressure is difficult to be directly measured. The characteristic relaxation time is the general variable detected in experiments and simulations. Based on Eq. 2.51 one can derive the relation between the relaxation time and the phonon gas pressure

$$\tau_R = \frac{\kappa}{c^2 dp_h/dT} \quad (2.62)$$

For the silicon at 300 K, with the properties chosen as $\kappa = 149 \text{ W m}^{-1} \text{ K}^{-1}$, $C_v = 704.6 \text{ J kg}^{-1} \text{ K}^{-1}$, $\rho = 2330 \text{ kg m}^{-3}$, $\gamma = 1.5$, the first algorithm gives a relaxation time of $1.4 \times 10^{-10} \text{ s}$, while the second algorithm yields $0.5 \times 10^{-10} \text{ s}$.

The experiments indicate that the relaxation time is 1.5×10^{-10} s [27]. Thus the results obtained through various methods are of the same magnitude.

The three terms on the left-hand side of Eq. 2.51 come from f_+ , f_{++} and f_0 respectively. If one only retains the third term, then Eq. 2.51 reduces to the Fourier's heat conduction law. If the terms from f_0 and f_+ are reserved, Eq. 2.51 transforms into the CV model describing the transient heat wave propagation. If all the three terms are fully considered, namely taking the second order expansion of the displaced Planck distribution, one obtains a governing equation similar to the momentum balance equation of phonon gas (Eq. 2.20). In ordinary cases, f_{++} is much smaller than f_0 and is thereby negligible. In extreme conditions such as high heat flux density, the contribution of f_{++} should be considered.

The second term on the left-hand side of Eq. 2.51 (convection term) has a coefficient 15/16. The corresponding term in the momentum balance equation of phonon gas should be unity (cf. Eq. 2.52). This distinction can be analyzed from the phonon energy variation caused by the Doppler Effect. Note that the coefficient 4/3 in Eq. 2.45 comes from the integration by parts

$$\begin{aligned}
 \int_k f_+^n \hbar \omega^n v_{kj} &= u_{Dj} \int_k f_0^n \hbar \omega^n + \int_k \hbar (\mathbf{k} \cdot \mathbf{u}_D) \frac{\partial \omega^n}{\partial k_j} f_0^n \\
 &= u_{Dj} \int_k f_0^n \hbar \omega^n + \frac{1}{3} u_{Dj} \int_k \hbar \omega^n f_0^n \\
 &= u_{Dj} \int_k f_0^n \hbar \omega^n + B u_{Dj} \int_k \hbar \omega^n f_0^n
 \end{aligned} \tag{2.63}$$

This integration assumes the cubic symmetry and agrees with Sussmann's results [20]. Equation 2.63 contains two parts. One is a uniform drift of the equilibrium part f_0 with a velocity u_{Dj} . The second part is induced by the derivative of the phonon energy, $\hbar \omega$, with respect to the wave vector k , which is measured by the coefficient B . The coefficient 15/16 in Eq. 2.51 is $(1 + 2B)/(1 + B)^2$, which is always less than unity. Therefore, this additional coefficient rises from the Doppler Effect during the drift motion of phonon gas. From this perspective, the phonon gas is slightly different from the real gas. The phonon energy varies due to dispersion causing the "eclipse" of the convection term. In a non-dispersive medium, the frequency is independent of k . In this case $B = 0$, and Eq. 2.51 will have exactly the same form as Eq. 2.52.

2.3.2 Chapman–Enskog Expansion

In Sect. 2.3.1 it is assumed that the phonon distribution function is approximated by f_D , which is reasonable only in pure crystals at low temperature. In other cases the

Umklapp scattering, impurity scattering, and other momentum breaking processes will continuously draw f away from f_D , which relaxes back to f_D with a relaxation time τ_N .

The second derivative of heat flux is proportional to τ_N in Eq. 1.7 with a scale coefficient $\tau_R \tau_N v_s^2/5$. When τ_R is much larger than τ_N , Eq. 2.32 can be written as

$$f_D^n - f^n = \tau_N (\partial/\partial t + \mathbf{v}_k \cdot \nabla) f^n \quad (2.64)$$

This form is close to Sussmann's assumption [22]. Since f_D can be regarded to represent the uniform drift motion of phonon gas, the second derivative term caused by τ_N thereby comes from the nonuniform motion of phonon gas. In this manner, the τ_N term in the Boltzmann equation gives the additional friction force induced by the local gradient of drift velocity. If one introduces a heterogeneous term into the thermomass pressure (Eq. 2.17) or the phonon gas pressure (Eq. 2.53) in analogy with the shear stress elements, the second derivative of heat flux then emerges as the viscous dissipation term containing the Laplacian of velocity in Navier–Stokes equations.

For more general cases, Banach and Jiaung et al. [28, 29] solved the phonon Boltzmann equation with the Chapman–Enskog expansion. The common points of these methods are: (1) The phonon distribution function is expressed by an expansion around f_D

$$f = f_D + Kn f_1 + Kn^2 f_2 + \dots \quad (2.65)$$

where Kn is the Knudsen number, which is the ratio of the average mean free path of particles over the characteristic size of flow region. (2) The first order Chapman–Enskog expansion f_1 is proportional to τ_N . (3) The first order Chapman–Enskog expansion will lead the second order derivative of heat flux in the governing equation. This is similar to the basic assumption in the derivation of Navier–Stokes equations.

Sussmann and Thellung [22] assumed that the phonon distribution function has the form

$$f = f_D - \tau_N (\partial/\partial t + \mathbf{v}_k \cdot \nabla) f_D \quad (2.66)$$

It also satisfies the three essential features of Chapman–Enskog expansion.

Without the Chapman–Enskog expansion, Banach et al. [28] obtained the governing equation of heat conduction in three-dimensional space as

$$\frac{\partial q_i}{\partial t} + \frac{1}{3} \nabla_j \int_k f_0^n \hbar \omega (v_k^n)^2 + \nabla_j M^{ij} = -\frac{q_i}{\tau_R} \quad (2.67)$$

where the zeroth order approximation of M_{ij} satisfies

$$M_0^{ij} = \frac{3}{2e + \sqrt{4e^2 - 3|\mathbf{q}|^2 / (v_k^n)^2}} \left(q_i q_j - \frac{1}{3} \delta_{ij} \right) \quad (2-68)$$

The drift velocity of phonon gas, u_h , is usually small. Therefore, $(q/v_s)^2$ is negligible compared with $4e^2$. Compared with Eq. 2.49, Eq. 2.67 can transform to

$$\frac{\partial q_i}{\partial t} + \frac{3}{4} \nabla_j \frac{q_i q_j}{e} + \frac{1}{3} \nabla_j \int_k f_0^s \hbar \omega (v_k^n)^2 = -\frac{q_i}{\tau_R} \quad (2.69)$$

Equation 2.69 has the same structure as Eq. 2.51, with the only difference in the coefficient of the convection term. This distinction is caused by overestimation of the Doppler effect during integration.

Therefore, one can conclude that the second order derivative term rises from the Chapman–Enskog expansion around f_D . The magnitude of Chapman–Enskog expansion is proportional to Kn. So this effect should be considered in the condition of large Kn, for e.g., the heat conduction in nanosystems.

2.3.3 Eigenvalue Analysis

The eigenvalue analysis has been used to solve the phonon Boltzmann equation by Guyer and Krumhansl [20] and Hardy [23]. The phonon distribution function is converted into symmetry form

$$f^*(\mathbf{k}, x, t) = f(\mathbf{k}, x, t) 2 \sin h \left(\frac{1}{2} x_k \right), \quad (2.70)$$

where

$$x_k = \frac{\hbar \omega}{k_B T} \quad (2.71)$$

With this the phonon Boltzmann equation (Eq. 2.27) turns to

$$Df^* = (R^* + N^*)f^* \quad (2.72)$$

It is assumed that the zero subspace of N^* has four and only four eigenvectors

$$\begin{aligned}
 |\eta_0\rangle &= \mu x_k \left(2 \sinh \frac{1}{2} x_k \right)^{-1} \\
 |\eta_{1x}\rangle &= \lambda_x q_x \left(2 k_B T \sinh \frac{1}{2} x_k \right)^{-1} \\
 |\eta_{1y}\rangle &= \lambda_y q_y \left(2 k_B T \sinh \frac{1}{2} x_k \right)^{-1} \\
 |\eta_{1z}\rangle &= \lambda_z q_z \left(2 k_B T \sinh \frac{1}{2} x_k \right)^{-1}
 \end{aligned} \tag{2.73}$$

These four eigenvectors correspond to the internal energy and the heat flux in three directions in a Cartesian coordinate system. $|\eta_0\rangle$ is the eigenvector of the zero subspace of both N^* and R^* . $|\eta_{1x}\rangle$, $|\eta_{1y}\rangle$ and $|\eta_{1z}\rangle$ are only the eigenvectors of the zero subspace of N^* but do not belong to the zero subspace of R^* , because R^* is the momentum breaking operator that does not conserve the quasi-momentum. Assuming that all other eigenvectors have nonzero eigenvalues, f^* can be written as the linear combination of the eigenvectors of N^* , which give the solution of the phonon Boltzmann equation

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{1}{3} (v_s)^2 \nabla E = - \frac{\mathbf{q}}{\tau_R} + \frac{\tau_N (v_s)^2}{5} (\nabla^2 + \zeta \nabla \nabla \cdot) \mathbf{q}, \tag{2.74}$$

where $\zeta = 2$ in [20] while $\zeta = 1/3$ in [23]. The second order derivative comes from the eigenvectors with nonzero eigenvalues. For $\beta = 1, 2, 3$, the expansions of the phonon distribution function around f_D is

$$\sum_{\alpha=0}^3 \sum_{\sigma \geq 4} \sum_{\mu \geq 4} \frac{\langle \beta | \mathbf{D} + \mathbf{R} | \sigma \rangle \langle \mu | \mathbf{D} + \mathbf{R} | \alpha \rangle}{N^\mu} f_\alpha, \tag{2.75}$$

where $\langle \alpha | \mathbf{D} + \mathbf{R} | \beta \rangle$ is the matrix element of the eigenvalues of $\mathbf{D} + \mathbf{R}$, N^μ denotes the μ th eigenvalue of the normal process collision matrix, and \mathbf{R} is the resistive collision operator. Since the drift operator \mathbf{D} contains the first order derivative of space, Eq. 2.75 introduces the second order derivative term in the governing equation. If the eigenvectors $|\sigma\rangle$ and $|\mu\rangle$ have zero eigenvalues, the second order derivative will vanish simultaneously. Therefore, Eq. 2.75 indicates that existence of the second order derivative in the governing equation requires that all the eigenvectors except $|\eta_0\rangle$, $|\eta_{1x}\rangle$, $|\eta_{1y}\rangle$ and $|\eta_{1z}\rangle$ should have nonzero eigenvalues with respect to $\mathbf{D} + \mathbf{R}$.

The phonon distribution function is approximated by f_D in Sect. 2.3.1. Based on Krumhansl's transformation [30], the first order expansion of f_D , namely $f_0 + f_+$, is one of the eigenvectors of the zero subspace of N . In this sense, if $|\eta_{1x}\rangle$, $|\eta_{1y}\rangle$ and $|\eta_{1z}\rangle$ are strictly proportional to the heat flux, they will have small but nonzero eigenvalues.

If their eigenvalue is strictly zero, they should contain the higher order term of heat flux. If the higher order terms of heat flux are considered in $|\eta_{1x}\rangle$, $|\eta_{1y}\rangle$ and $|\eta_{1z}\rangle$, it will introduce the convection term in the governing equation of phonon gas dynamics. This is the reason for the distinction between Eqs. 2.51 and 2.74.

2.4 Conclusion

Based on Einstein's mass energy equivalence, the thermal energy stored in the medium contributes to its rest mass, namely the thermomass. The thermomass is a real mass. It has the inertia and gravity effects. The thermomass moves relatively to the rest lattices in heat conduction. The mass flow rate of thermomass corresponds to the heat flux. Based on the generalized mass flux and momentum flux, it can be derived that the motion of thermomass satisfies Newton's law of motion as long as the conduction medium and the thermomass move much slower than the speed of light.

Phonons are the main heat carriers in dielectric solids. The aggregate of phonons in pure dielectric crystals can be regarded as a phonon gas. The dynamic variables such as the equation of state, density, drift velocity, and momentum of phonon gas can be derived from the thermomass theory. The balance equations of the mass and momentum of phonon gas lead to the energy conservation relation and the general heat conduction law. In bulk materials, the friction force on the phonon gas obeys the Darcy's law, i.e., proportional to the drift velocity of phonon gas. The viscosity of phonon gas causes the boundary to additionally impede the phonon gas in nanosystems. In this case the friction force on the phonon gas contains not only the Darcy term proportional to the drift velocity but also the Brinkman term proportional to the second order derivative of the drift velocity.

The dynamic governing equations of phonon gas can be microscopically derived based on the phonon Boltzmann equation. When the relaxation time of R processes is much larger than that of N processes, the phonon distribution function can be approximated by the displaced Planck distribution, f_D . When only the zeroth order of f_D is considered, the Boltzmann equation will give the traditional Fourier's law. Considering the first order expansion of f_D will give the CV model. If the second order of expansion is reserved, one obtains the momentum balance equation phonon gas containing the convection term, which agrees with the macroscopic derivation based on the thermomass theory (Eq. 2.20). If the relaxation time of R processes is not big enough, then the Chapman–Enskog expansion can be implemented around f_D . In this case the second order derivative of heat flux will be introduced into the heat conduction equation. The eigenvalue analysis also obtains the second order derivative of heat flux. However, it assumes there are only four eigenvectors in the zero subspace of N operator, which resultantly eliminates the convection term in the heat conduction equation.

References

1. Moller C (1972) The theory of relativity. Clarendon Press, Oxford
2. Misner CM (1973) Gravitation. WH Freeman and Company, San Francisco
3. Schroder UE (1990) Special relativity. World Scientific, Singapore
4. Rindler W (1982) Introduction to special relativity. Clarendon Press, Oxford
5. Einstein A, Infeld L (1938) The evolution of physics: the growth of ideas from early concepts to relativity and quanta. Simon and Schuster, New York
6. Taylor EF, Wheeler JA (1966) Spacetime physics. W.H. Freeman and Company, New York
7. Kittel C (1996) Introduction to solid state physics, 7th edn. Wiley, New York
8. Reissland JA (1973) The physics of phonons. Wiley, London
9. Guo ZY, Cao BY, Zhu HY et al (2007) State equation of phonon gas and conservation equations for phonon gas motion. *Acta Phys Sin* 56(6):3306–3312
10. Guo ZY, Cao BY (2008) A general heat conduction law based on the concept of motion of thermal mass. *Acta Phys Sin* 57(7):4273–4281
11. Cao BY, Guo ZY (2007) Equation of motion of a phonon gas and non-Fourier heat conduction. *J Appl Phys* 102(5):053503
12. Tzou DY, Guo ZY (2010) Nonlocal behavior in thermal lagging. *Int J Therm Sci* 49(7):1133–1137
13. Guo ZY, Hou QW (2010) Thermal wave based on the thermomass model. *J Heat Transfer* 132(7):072403
14. Wang M, Guo ZY (2010) Understanding of temperature and size dependences of effective thermal conductivity of nanotubes. *Phys Lett A* 374(42):4312–4315
15. Wang M, Yang N, Guo ZY (2011) Non-Fourier heat conductions in nanomaterials. *J Appl Phys* 110(6):064310
16. Wang M, Shan X, Yang N (2012) Understanding length dependences of effective thermal conductivity of nanowires. *Phys Lett A* 376(46):3514–3517
17. Wang HD, Cao BY, Guo ZY (2010) Heat flow choking in carbon nanotubes. *Int J Heat Mass Transf* 53(9):1796–1800
18. Christov CI, Jordan PM (2005) Heat conduction paradox involving second-sound propagation in moving media. *Phys Rev Lett* 94:154301
19. Müller I, Ruggeri T (1993) Extended thermodynamics. Springer, New York
20. Guyer RA, Krumhansl JA (1966) Solution of the linearized phonon Boltzmann equation. *Phys Rev* 148(2):766–778
21. Guyer RA, Krumhansl JA (1966) Thermal conductivity, second sound, and phonon hydrodynamic phenomena in nonmetallic crystals. *Phys Rev* 148(2):778
22. Sussmann JA, Thellung A (1963) Thermal conductivity of perfect dielectric crystals in the absence of umklapp processes. *Proc Phys Soc* 81(6):1122
23. Hardy RJ (1970) Phonon Boltzmann equation and second sound in solids. *Phys Rev B* 2(4):1193
24. Hardy RJ, Albers DL (1974) Hydrodynamic approximation to the phonon Boltzmann equation. *Phys Rev B* 10(8):3546
25. Gurevich VL (1986) Transport in phonon systems. North-Holland, Amsterdam
26. Enz CP (1968) One-particle densities, thermal propagation, and second sound in dielectric crystals. *Ann Phys* 46(1):114–173
27. Sahasrabudhe GG, Lambade SD (1999) Temperature dependence of the collective phonon relaxation time and acoustic damping in Ge and Si. *J Phys Chem Solids* 60(6):773–785
28. Banach Z, Larecki W (2008) Chapman-Enskog method for a phonon gas with finite heat flux. *J Phys A Math Theor* 41(37):375502

29. Jiaung WS, Ho JR (2008) Lattice-Boltzmann modeling of phonon hydrodynamics. *Phys Rev E* 77(6):066710
30. Krumhansl JA (1965) Thermal conductivity of insulating crystals in the presence of normal processes. *Proc Phys Soc* 85(5):921

Dynamical Analysis of Non-Fourier Heat Conduction and
Its Application in Nanosystems

Dong, Y.

2016, XVIII, 134 p., Hardcover

ISBN: 978-3-662-48483-8