Generalized heat conduction laws based on thermomass theory and phonon hydrodynamics

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The Fourier's law of heat conduction is invalid in extreme conditions, such as the second sound in solids and anomalous heat conduction in nanosystems. The generalized heat conduction law with nonlinear and nonlocal effects is derived from both macroscopic thermomass theory and microscopic phonon Boltzmann method in this paper. The coincidence between thermomass theory and phonon hydrodynamics is also analyzed through their microscopic basis. The convective term in the momentum equation of the thermomass theory comes from the nonlinear terms of the distribution function, which is often neglected in previous phonon hydrodynamics derivations. The Chapman-Enskog expansion leads to the Laplacian term, which is similar to the derivation of Navier-Stokes equation in hydrodynamics and inspires the introduction of a Brinkman extension in the thermomass equation. This comparison reveals how the nonlinear effects could be described by generalized heat conduction laws. © *2011 American Institute of Physics*. [doi:10.1063/1.3634113]

I. INTRODUCTION

Generally, thermal transport in materials is described by the Fourier's law of heat conduction, which is applicable for most practical situations. However, for fast-transient heat conduction, the temperature evolution equation based on the Fourier's law is parabolic and predicts an infinite speed of heat propagation. Therefore, the Fourier's law of heat conduction breaks down in modeling laser processing of materials[1,2] or high frequency response in IC chips,[3] where heat propagates as thermal waves. On the other hand, the thermal transport in nanostructure materials, such as nanowires and nano-films, are quite different from the bulk ones. The low dimensional materials, such as carbon nano-tubes (CNTs)[4–6] and single-layer graphene[7] show ultrahigh thermal conductivities, while some others show decreased thermal transport properties compared with bulk materials, due to boundary scattering or confinement of lattice waves.[8–11] The size dependent effective thermal conductivity cannot be described by the Fourier's conduction law, so a generalized heat conduction law is highly required.

From a microscopic point of view, the finite propagation speed of heat should be attributed to the fact that energy carriers move with a limited speed. The Fourier's law is only an approximate description, neglecting the time needed for acceleration of energy carriers.[12] Specifically, the thermal energy in dielectric solids is carried by phonons, which are the quantization of the modes of lattice vibrations. Therefore, the heat conduction equation can be derived from the phonon state distribution function in non-equilibrium systems. In the theory of phonon hydrodynamics,[13–22] a set of non-Fourier heat conduction laws have been obtained through solving the phonon Boltzmann equation. The forms of these conduction laws are similar to the hydrodynamic governing equations. The time relaxation term is included and predicts the finite propagation speed of thermal disturbance. The heat flow through a nanowire is analogous to the viscous Poiseuille flow passing through a tube, so the reduction of effective heat conductivity of nanowires is explained by the boundary drag. Similar transport equations were derived macroscopically by the extended irreversible thermodynamics (EIT)[23–29] and used to investigate the heat conduction in nanowires.

The thermomass theory also proposes a hydrodynamic-like description of heat conduction.[30–37] The thermal energy has an equivalent mass (thermomass) according to Einstein's theory of special relativity, which should be seen as a part of the invariant mass of the system in modern physics.[38–40] The nonlocal and nonlinear effects of heat conduction can be ascribed to the inertia of thermomass. The governing equation based on the thermomass model predicts the wave-like heat transport in transient condition and the variation of effective thermal conductivity with temperature and size of nanowires at steady state, which agrees with the experimental results.[37] The governing equations derived from the thermomass model are also found to be similar to those based on phonon hydrodynamics and EIT.[26] In this paper, we investigate the coincidences between the thermomass model and phonon hydrodynamics by analysis on the solution of the phonon Boltzmann equation. The comparison and combination of different theories are expected to deepen the knowledge of heat conduction in phonon systems.

II. THERMOMASS EQUATION WITH BRINKMAN EXTENSION

In the thermomass theory, the thermal energy in media has an equivalent mass defined by the Einstein's mass-energy equivalence relation, and the motion of the thermomass can be described by Newton's mechanics.[30–37] The density of the thermomass contained in the media is

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$$\rho_{\rm h} = \frac{\rho C_V T}{c^2}, \tag{1}$$

where $\rho C_{\rm v} T$ represents the thermal energy density and c is the speed of light in vacuum. The thermomass density, $\rho_{\rm h}$, has a unit of kg·m^{-3}. The drift velocity of the thermomass $\boldsymbol{u}_{\rm h}$ is defined as

$$\boldsymbol{u}_{\rm h} = \frac{\boldsymbol{q}}{\rho C_V T}, \tag{2}$$

where $\boldsymbol{q}$ is the heat flux vector. The governing equation of heat conduction could be obtained in analogy with hydrodynamics

$$\frac{\partial \rho_{\rm h}}{\partial t} + \nabla \cdot (\rho_{\rm h} \boldsymbol{u}_{\rm h}) = 0, \tag{3}$$

$$\rho_{\rm h} \frac{\partial \boldsymbol{u}_{\rm h}}{\partial t} + (\rho_{\rm h} \boldsymbol{u}_{\rm h} \cdot \nabla) \boldsymbol{u}_{\rm h} + \nabla \cdot \Pi = 0, \tag{4}$$

where $\boldsymbol{\Pi}$ is the stress tensor, and the body force is neglected. Equation (3) gives the energy conservation relation when Eqs. (1) and (2) are substituted into it. We temporarily assume that the thermomass bears a friction in its flow region, as the Darcy flow in porous hydrodynamics, and ignore the deviatoric stress tensor; thus, the momentum conservation in Eq. (4) can be written as

$$\rho_{\rm h} \frac{\partial \boldsymbol{u}_{\rm h}}{\partial t} + (\rho_{\rm h} \boldsymbol{u}_{\rm h} \cdot \nabla) \boldsymbol{u}_{\rm h} + \nabla p_{\rm h} = \boldsymbol{f}_{\rm h}. \tag{5}$$

The unknown isotropic part of the stress tensor falls into a simple form based on the Debye state equation

$$p_{\rm h} = \gamma \rho_{\rm h} C_V T = \frac{\gamma \rho (C_V T)^2}{c^2}, \tag{6}$$

where γ is the Grüneisen parameter. The Darcy's law is applied to give the expression of $\boldsymbol{f}_{\rm h}$, i.e., the friction is proportional to the drift velocity $\boldsymbol{u}_{\rm h}$. Since the steady heat conduction obeys the Fourier's law in bulk materials, in this situation, Eq. (5) turns out to be the balance of driving force and friction force, i.e.,

$$\nabla p_{\rm h} = \boldsymbol{f}_{\rm h}. \tag{7}$$

Comparing Eq. (7) with the Fourier's law, the friction term appears as[30]

$$\boldsymbol{f}_{\rm h} = -\beta \boldsymbol{u}_{\rm h} = -\frac{2\gamma C_V (\rho C_V T)^2}{\kappa c^2} \boldsymbol{u}_{\rm h}, \tag{8}$$

where β is the friction coefficient and κ is the thermal conductivity of bulk materials. In this way, the generalized heat conduction equation is given:

$$\tau_{\rm TM} \frac{\partial \boldsymbol{q}}{\partial t} + 2\mathbf{l} \cdot \frac{\partial \boldsymbol{q}}{\partial x} - b\kappa \nabla T + \kappa \nabla T + \boldsymbol{q} = 0, \tag{9}$$

where

$$\tau_{\rm TM} = \frac{\kappa}{2\gamma \rho C_V^2 T}, \tag{10a}$$

$$\boldsymbol{l} = \frac{\boldsymbol{q}\kappa}{2\gamma C_V (\rho C_V T)^2} = \boldsymbol{u}_{\rm h} \tau_{\rm TM}, \tag{10b}$$

$$b = \frac{q^2}{2\gamma \rho^2 C_V^3 T^3} = Ma_{\rm h}^2, \tag{10c}$$

with $\tau_{\rm TM}$ being the lagging time, $\boldsymbol{l}$ the length vector, and $Ma_{\rm h}$ the Mach number of the drift velocity, $u_{\rm h}$, relative to the thermal wave speed in the phonon gas, $u_{\rm hs}$. The first three terms on the left-hand side of Eq. (9) result from the inertia effects. The fourth term represents the effect from the pressure gradient (driving force), and the last term denotes the resistance as the phonon gas flows through the lattice. Equation (9) reduces to the C-V equation with the second and third inertia terms ignored. Cimmelli *et al.*[24,25] obtained a similar governing equation to Eq. (9) based on a dynamical nonequilibrium temperature. In their paper, the effect described by the second and third inertia terms in Eq. (9) has a coincident counterpart.

Although Eq. (9) gives a porous hydrodynamic equation for heat conduction, the boundary effects become important in nanosystems. A Brinkman term was introduced to the traditional form of Darcy's law when transitional flow between boundaries should be taken into account.[41] In analogy with this extension in porous hydrodynamics, the thermomass governing equation can be modified to

$$\tau_{\rm TM} \frac{\partial \boldsymbol{q}}{\partial t} + 2l \nabla \boldsymbol{q} - b\kappa \nabla T + \kappa \nabla T + \boldsymbol{q} - \mu \nabla^2 \boldsymbol{q} = 0, \tag{11}$$

where μ is the effective viscosity of the thermomass and determined by the thermal properties. In porous media, the Brinkman extension predicts a boundary layer, wherein the nonslip or slip boundary condition changes the drift velocity significantly. However, this boundary layer is usually very thin and can be ignored in large scale systems. Similarly, the Brinkman term in Eq. (11) exhibits additional drag by the walls of the system and should be considered for nanoscale systems in which the characteristic length of the system is comparable with the friction boundary layer of the thermomass. In other words, the Brinkman extension is necessary only if the Knudsen number of the system is large enough. This extension has also been suggested by Ref. 26 to show an illustrative and interesting similarity to the nonlinear extension of the Guyer-Krumhansl (GK) equation, and the effective viscosity μ is related to the square of mean free path of the energy carriers (see Eq. (1) in Ref. 26).

III. PHONON BOLTZMANN DERIVATION

The phonon hydrodynamics can give generalized heat conduction laws through solving the phonon Boltzmann equation.[13–22] Generally, the target is to search the real phonon distribution function f and, thus, the governing equations can be obtained. However, many assumptions are required to solve the Boltzmann equation, as in fluid mechanics. Different approaches dealing with the Boltzmann equation lead to different governing equations. In the following section, the Boltzmann equation will be analyzed with the concept of thermomass and compared with other solutions in terms of phonon hydrodynamics. This will show the inherent similarity between the governing equations for heat conduction based on thermomass theory and that based on the phonon hydrodynamics.

The phonon Boltzmann equation focuses on the distribution function of phonons to describe its deviation by operators as

$$\boldsymbol{D}f(\boldsymbol{k},\boldsymbol{x},t)=\boldsymbol{C}f(\boldsymbol{k},\boldsymbol{x},t), \quad (12)$$

where $\boldsymbol{D}$ and $\boldsymbol{C}$ are the drift and collision operators, respectively. The macroscopic variables, such as internal energy density E and heat flux $\boldsymbol{q}$, are related to the microscopic distribution function as[19–22]

$$E=\sum_s\int_{\mathbf{k}}\hbar\omega_s f_s, \quad (13)$$

$$q_i=\sum_s\int_{\mathbf{k}}\hbar\omega_s\frac{\partial\omega_s}{\partial k_i}f_s, \quad (14)$$

where s is the index of phonon branches, $\boldsymbol{k}$ is the wave vector, and ω is the frequency. The integral is over the whole $\boldsymbol{k}$ space and then summed over all branches. Sussmann *et al.*[15] deduced a heat conduction equation by neglecting the Umklapp processes in perfect dielectric crystals by a mean free time approximation on the distribution function. Guyer *et al.*[18] carried out an eigenvalue analysis of Eq. (12) to obtain a comprehensive governing equation as the Guyer-Krumhansl equation

$$\tau_R\frac{\partial\boldsymbol{q}}{\partial t}+\boldsymbol{q}=-\kappa\nabla T+l^2\left(\nabla^2\boldsymbol{q}+2\nabla\nabla\cdot\boldsymbol{q}\right), \quad (15)$$

where ℓ is the mean free path of phonons. The form of Eq. (15) is similar to Sussmann *et al.*'s results[15] and it is further discussed by Hardy *et al.*[20] The impact on heat conduction of Umklapp scattering and other quasi-momentum non-conserving processes in Eq. (15) is described by a relaxation time τ_R.

The distribution function for equilibrium state follows the Planck distribution

$$f_E=\frac{1}{\exp(\hbar\omega/k_BT)-1}. \quad (16)$$

The normal process tends to relax the distribution function to the displaced Planck distribution[13–15]

$$f_D=\frac{1}{\exp[(\hbar\omega-\hbar\boldsymbol{k}\cdot\boldsymbol{u})/k_BT]-1}, \quad (17)$$

where $\boldsymbol{u}$ is the so-called drift velocity of the phonon gas. The resistive quasi-momentum non-conserving process tends to relax the distribution function to the equilibrium Planck distribution f_E. Thus, a relaxation type of phonon Boltzmann Eq. (12) can be written as[21,22]

$$\left(\frac{\partial}{\partial t}+\boldsymbol{v}^s\cdot\nabla\right)f^s=\frac{f_E^s-f^s}{\tau_R}+\frac{f_D^s-f^s}{\tau_N}, \quad (18)$$

where $\boldsymbol{v}$ is the group velocity and t_N is the relaxation time of the normal process.

In low temperature perfect crystals, the normal processes are dominant and the Umklapp processes are rare, so $\tau_N \ll \tau_R$; then f_D is a good approximation to the real distribution.[13–15] This is the simplest assumption to demonstrate the structure of the solution of the Boltzmann equation. The deviation from f_D could be taken into account by a Chapman-Enskog expansion, which will be discussed in detail in Sec. IV A.

Substituting f_D into Eq. (18) gives

$$\left(\frac{\partial}{\partial t}+\boldsymbol{v}^s\cdot\nabla\right)f_D^s=\frac{f_E^s-f_D^s}{\tau_R}. \quad (19)$$

To obtain a transport governing equation, Eq. (19) could be multiplied with $\hbar k_i$ or $\hbar\omega v_i$ to lead to the drifting or driftless second sound, respectively.[19] The difference between the two kinds of second sound could be seen from the equation (cf. Eq. (28) in Ref. 20)

$$\frac{v'_{\rm II}}{v_{\rm II}}=\frac{\sum_{{\rm all}\,\sigma}\langle 0|v^1|\sigma\rangle\langle\sigma|v^1|0\rangle}{\sum_{\sigma=0}^{3}\langle 0|v^1|\sigma\rangle\langle\sigma|v^1|0\rangle}, \quad (20)$$

where $\langle\alpha|\mathbf{v}|\beta\rangle$ is the matrix element of the group velocity in the eigenvector representation, $v_{\rm II}$ and $v'_{\rm II}$ are, respectively, the velocities of drifting and driftless second sound. Thus, the treatment leading to the driftless second sound is more comprehensive. It was addressed by Hardy[19] 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."

According to thermomass theory, the second method is preferable. In the transport theory for gases,[42] multiplying the Boltzmann equation by the momentum of molecules mv gives the momentum conservation equation. In phonon gases, $\hbar\omega$ is the energy of a phonon and $\hbar\omega/c^2$ is the equivalent mass according to the thermomass theory. In this way, $\hbar\omega v_i/c^2$ presents the collective momentum of the phonon gas induced by heat flux. It is the real momentum and different from the quasi-momentum of phonons, i.e., $\hbar k$. Multiplying Eq. (19) by $\hbar\omega/c^2$ and $\hbar\omega v_i/c^2$ would lead to the mass and momentum conservation equation for phonon gases, as in hydrodynamics.[42] However, unlike ideal gases in channels, the phonon gases bear the resistance from the Umklapp processes or crystal defects. This difference is reflected by a sink term of the momentum when the collision term in Eq. (19) is multiplied by $\hbar\omega v_i/c^2$. In practice, the parameter c^2 could be canceled out from the equations since it is a constant.

Multiplying Eq. (19) by $\hbar\omega$ and $\hbar\omega v_i$, respectively, and integrating it in k space yields

$$\frac{\partial\int_k f_D^s\hbar\omega}{\partial t}+\int_{\mathbf{k}}\boldsymbol{v}^s\cdot\nabla f_D^s\hbar\omega=\frac{\int_{\mathbf{k}}(f_E^s-f_D^s)\hbar\omega}{\tau_R}, \quad (21)$$

$$\frac{\partial\int_{\mathbf{k}} f_D^s\hbar\omega v_i}{\partial t}+\int_{\mathbf{k}}\boldsymbol{v}^s\cdot\nabla f_D^s\hbar\omega v_i=\frac{\int_{\mathbf{k}}(f_E^s-f_D^s)\hbar\omega v_i}{\tau_R}. \quad (22)$$

When the drift velocity $\boldsymbol{u}$ is small, a Taylor expansion of f_D around equilibrium up to second order could be deduced as

$$f_{\rm D} = f_{\rm E} + \frac{\partial f_D}{\partial \mathbf{u}}\bigg|_{\Delta u=0}\Delta\mathbf{u} + \frac{1}{2}\frac{\partial^2 f_{\rm D}}{\partial \mathbf{u}^2}\bigg|_{\Delta u=0}(\Delta\mathbf{u})^2 + o\Big((\Delta\mathbf{u})^2\Big)$$
$$= f_{\rm E} + \frac{\partial f_{\rm E}}{\partial \omega}(\mathbf{k}\cdot\mathbf{u}) + \frac{1}{2}\frac{\partial^2 f_{\rm E}}{\partial \omega^2}(\mathbf{k}\cdot\mathbf{u})^2 + o\Big((\Delta\mathbf{u})^2\Big)$$
$$= f_{\rm E} + f_+ + f_{++} + o\Big((\Delta\mathbf{u})^2\Big), \tag{23}$$

where $f_{\rm E}$ and f_{++} are even functions in k space while f_+ is odd. Substituting the second order expansion of $f_{\rm D}$ into Eqs. (21) and (22) gives

$$\frac{\partial \int_k (f_{\rm E}^s + f_{++}^s)\hbar\omega}{\partial t} + \nabla_j \int_k f_+^s \hbar\omega v_j = -\frac{\int_k f_{++}^s \hbar\omega}{\tau_{\rm R}}, \tag{24}$$

$$\frac{\partial \int_k f_+^s \hbar\omega v_i}{\partial t} + \nabla_j \int_k (f_{\rm E}^s + f_{++}^s)\hbar\omega v_i v_j = -\frac{\int_k f_+^s \hbar\omega v_i}{\tau_{\rm R}}. \tag{25}$$

The integral in the second term in Eq. (24) could be expressed explicitly through integration by parts

$$\int_{\mathbf{k}} f_+^s \hbar\omega v_j = \frac{4}{3}u_j \int_{\mathbf{k}} f_E^s \hbar\omega = \frac{4}{3}u_j E = q_j. \tag{26}$$

Since f_{++} should be much smaller than $f_{\rm E}$, its contribution to the internal energy is reasonably omitted. In addition, $\tau_{\rm R}$ is large compared with the characteristic time of evolution. On the other hand, $\hbar\omega$ is the summational invariant of the Boltzmann equation, since the collision term conserves energy. Then, Eq. (24) yields

$$\frac{\partial E}{\partial t} + \nabla_j q_j = 0, \tag{27}$$

which is the energy balance relation. The integral in the second term in Eq. (25) could be divided into an equilibrium part and a dynamical part

$$\int_{\mathbf{k}} (f_{\rm E}^s + f_{++}^s)\hbar\omega v_i v_j = \delta_{ij}\int_{\mathbf{k}} f_{\rm E}^s \hbar\omega v_i v_j + \int_{\mathbf{k}} f_{++}^s \hbar\omega v_i v_j. \tag{28}$$

The second term in Eq. (28) could be integrated by parts

$$\int_{\mathbf{k}} f_{++}^s \hbar\omega v_i v_j = \frac{5}{3}u_i u_j E. \tag{29}$$

Using all these results in Eqs. (26), (28), and (29), the governing equation from Eq. (25) turns out to be

$$\frac{\partial q_i}{\partial t} + \frac{15}{16}\nabla_j \frac{q_i q_j}{E} + \frac{1}{3}\nabla_j \int_{\mathbf{k}} f_E^s \hbar\omega (v^s)^2 = -\frac{q_i}{\tau_R}. \tag{30}$$

The third term in the left-hand side of Eq. (30) assumes a cubic symmetry condition.

The momentum transport Eq. (30) could be compared with that in the thermomass theory

$$\frac{\partial q_i}{\partial t} + \nabla_j \frac{q_i q_j}{E} + \nabla_i p_{\rm h} = -\beta \frac{q_i}{E}, \tag{31}$$

where β is the friction coefficient [cf. Eq. (8)]. Equation (31) has been modified by adding the thermomass conservation relation Eq. (3) to show a parallel form with Eq. (30). The isotropic thermomass pressure is presented in the phonon Boltzmann method as

$$p_{\rm h} = \frac{1}{3}\int_k f_{\rm E}^s \frac{\hbar\omega}{c^2}(v^s)^2 = \iiint_{\pm\pi/a} f_{\rm E}^s(\boldsymbol{x}, t, \boldsymbol{k})\frac{\hbar\omega}{c^2} v_x^2 {\rm d}k_x {\rm d}k_y {\rm d}k_z. \tag{32}$$

It is interesting to notice that, in the kinetic theory of gases, the pressure in x direction is

$$p_x = \iiint_{\pm\infty} f(\boldsymbol{x}, t, \boldsymbol{v}) m v_x^2 {\rm d}v_x {\rm d}v_y {\rm d}v_z, \tag{33}$$

where p is the thermodynamic pressure, f is the localized distribution function, m is the mass of molecule, and $\boldsymbol{v}$ is the molecular velocity. Equations. (32) and (33) are actually the same in physical meaning. The temperature gradient driving the heat flux corresponds to the pressure gradient of the heat carriers, just as in hydrodynamics. The phonon gas pressure can be obtained either macroscopically by Eq. (6) or microscopically by Eq. (32). The predicted relaxation time for Si at 300 K, based on the first method, is calculated to be 1.4×10^{-10} s when the material properties are selected as: $\kappa = 149$ W m^{-1} K^{-1}, $C_{\rm v} = 704.6$ J kg^{-1} K^{-1}, $\rho = 2330$ kg m^{-3}, and $\gamma = 1.5$.[43] The second method predicts the thermal relaxation time to be 0.5×10^{-10} s (calculated by Ref. 44). The experimental value reported by Ilisavskii and Sternin[44] is about 1.5×10^{-10} s. This comparison shows that the results from both methods are of the same order of magnitude.

It should be noticed that the three terms on the left-hand side of Eq. (30) comes from f_+, f_{++}, and $f_{\rm E}$, respectively. If only the third term is reserved, it reduces to the traditional Fourier's law of heat conduction, i.e., Eq. (1). If the terms from $f_{\rm E}$ and f_+ are reserved, it gives the telegraphic Cattaneo-Vernotte thermal wave equation, i.e., Eq. (2). The displaced Planck distribution, when expanded to the second order, gives a governing equation through solving the Boltzmann equation similar to the thermomass theory.

However, the coefficient of the convective term is 15/16 in Eq. (30), while unity in Eq. (32). This can be analyzed by the change of the phonon energy caused by the Doppler effect. Specifically, there is a parameter 4/3 in Eq. (26), which comes from the process of integrating by parts

$$\int_{\mathbf{k}} f_+^s \hbar\omega v_j = u_j \int_k f_E^s \hbar\omega + \int_{\mathbf{k}} \hbar(\boldsymbol{k}\cdot\boldsymbol{u})\frac{\partial\omega}{\partial k_j} f_E^s$$
$$= u_j \int_{\mathbf{k}} f_E^s \hbar\omega + \frac{1}{3}u_j \int_{\mathbf{k}} \hbar\omega f_E^s \tag{34}$$
$$= u_j \int_{\boldsymbol{k}} f_E^s \hbar\omega + B u_j \int_{\boldsymbol{k}} \hbar\omega f_E^s.$$

This process assumes the cubic symmetry and agrees with Sussmann's integration.[15] It means that, besides a uniform motion of the equilibrium distribution function $f_{\rm E}$ with the drift velocity u_j (the first part of Eq. (34)), there is an additional part (measured by B) caused by the derivative of $\hbar\omega$ with respect to the wave vector $\boldsymbol{k}$. The parameter 15/16 in Eq. (30) is $(1+2B)/(1+B)^2$ and less than unity. This effect comes from the Doppler behavior of phonon gas during the drift motion, which is demonstrated by the second term in

Eq. (35). The phonon gas is different from the gas consisting of real particles, since the energy of phonon varies with the drift motion, so the convective term is "gibbous".

IV. COMPARISON WITH CHAPMAN-ENSKOG EXPANSION AND EIGEN ANALYSIS

A. Chapman-Enskog expansion

In Sec. III, the displaced Planck distribution is used to approximate the real distribution. However, it is reasonable only if the crystal is pure and kept at low temperature. The Umklapp processes and other scattering mechanism do not conserve the quasi-momentum of phonon gas,[13] so the real distribution deviates from the displaced Planck distribution and relaxes to f_D by a relaxation time τ_N.

In Guyer's paper,[18] the Laplacian term (second term on the right-hand side of Eq. (15)) is proportional to τ_N:

$$l^2 = \frac{\tau_N c_D^2}{5}, \tag{35}$$

where c_D is the Debye average velocity. When τ_R is large in Eq. (18), τ_N can be seen from

$$f_D - f = \tau_N(\partial/\partial t + \mathbf{v}\cdot\nabla)f, \tag{36}$$

which is close to that in Sussmann's paper (cf. Eq. (3) in Ref. 15). This variable indicates the relaxation time of the deviation of the real distribution from f_D. It could be recognized that f_D means a uniform drift of the phonon gas, so the Laplacian term in Eq. (15) comes from the non-uniform drift. Thus, the local drift velocity gradient will cause an additional resistance though the phonon Boltzmann equation. If the anisotropic part is introduced in the thermomass stress tensor $\mathbf{\Pi}$ in Eq. (4), it leads to the Laplacian term in Eq. (11), as in hydrodynamics.

In more general cases, Larecki and Jiaung *et al.*[21,22] have solved the phonon Boltzmann equation using the Chapman-Enskog expansion, as in hydrodynamics. It is common in their methods that: 1) The real distribution could be expressed by an expansion about the displaced Planck distribution:

$$f = f_D + \varepsilon f_1 + \varepsilon^2 f_2 + \ldots, \tag{37}$$

where ε is the Knudsen number and equals the ratio between the mean free path of a particle and the scale of variations of hydrodynamic fields. 2) The first order expansion f_1 is proportional to the relaxation time τ_N. 3) Because of the first order Chapman-Enskog expansion, a Laplacian term appears in the governing equation of the heat flux, just as that in hydrodynamics.[20] The results by Jiaung *et al.*[22] are consistent with Hardy's,[20] while the Larecki's[21] results are much more complicated.

Their results could be compared with Sussmann *et al.*,[15] where the real distribution is assumed to be

$$f = f_D - \tau_N(\partial/\partial t + \boldsymbol{v}\cdot\nabla)f_D. \tag{38}$$

This function satisfies the three features of Jiaung and Larecki's[21,22] method mentioned above.

It is observed that the three dimensional Larecki's governing equation without the Chapman-Enskog expansion is very similar to Eq. (30) [see Eq. (2.10c) in Ref. 21],

$$\frac{\partial q_i}{\partial t} + \frac{1}{3}\nabla_j\int_{\mathbf{k}} f_E^s \hbar\omega (v^s)^2 + \nabla_j M^{ij} = -\frac{q_i}{\tau_R}, \tag{39}$$

where the lowest approximation of M^{ij} is

$$M_0^{ij} = \frac{3}{2E + \sqrt{4E^2 - 3|\mathbf{q}|^2/(v^s)^2}}\left(q_i q_j - \frac{1}{3}\delta_{ij}\right). \tag{40}$$

Given the drift velocity u_h is small in ordinary cases and the isotropic trace of the second term in Eq. (28) has not been separated and added into the first term, Eq. (39) could be reformed as

$$\frac{\partial q_i}{\partial t} + \frac{3}{4}\nabla_j \frac{q_i q_j}{E} + \frac{1}{3}\nabla_j\int_{\mathbf{k}} f_E^s \hbar\omega (v^s)^2 = -\frac{q_i}{\tau_R}. \tag{41}$$

It is consistent with Eq. (30), except the coefficient of the second term.

Thus, it is confirmed that the Laplacian term in governing equations comes from the expansion around the displaced Planck distribution, which becomes important with a large Knudsen number for the heat conduction in nanosystems.

B. Eigen analysis of normal process collision matrix

Guyer, Krumhansl, and Hardy[18,20] solved the phonon Boltzmann equation by the method of Eigen analysis. They obtained the governing equation at low temperature and in dispersionless media:

$$\frac{\partial \boldsymbol{q}}{\partial t} + \frac{1}{3}(v^s)^2\nabla E = -\frac{\boldsymbol{q}}{\tau_R} + \frac{\tau_N (v^s)^2}{5}\left(\nabla^2 + \zeta\nabla\nabla\cdot\right)\boldsymbol{q}, \tag{42}$$

where ζ is 2 in Ref. 18 and 1/3 in Ref. 20, respectively. This discrepancy has been analyzed in Ref. 20. The four eigenvectors of the normal process collision matrix with vanishing eigenvalues are the single energy eigenvector f_0 and the three crystal momentum density eigenvectors f_1, f_2, and f_3. It is assumed that all other eigenvectors have non-vanishing eigenvalues. The Laplacian term in Eq. (42) comes from this assumption. For $\beta = 1$, 2, and 3, the last term in the governing equation for eigenvectors f is (see Eq. (15) in Ref. 20)

$$\sum_{\alpha=0}^{3}\sum_{\sigma\geq 4}\sum_{\mu\geq 4}\frac{\langle\beta|\boldsymbol{D}+\boldsymbol{R}|\sigma\rangle\langle\mu|\boldsymbol{D}+\boldsymbol{R}|\alpha\rangle}{N^\mu} f_\alpha, \tag{43}$$

where $\langle\alpha|\boldsymbol{D}+\boldsymbol{R}|\beta\rangle$ is the matrix element of the operator $\boldsymbol{D}+\boldsymbol{R}$ in the eigenvector representation, N^μ denotes the μth eigenvalue of the normal process collision matrix, and $\boldsymbol{R}$ is the resistive collision operator (including the Umklapp process and other momentum non-conservation processes). The drift operator $\boldsymbol{D}$ contains the spatial differential, so this term gives the Laplacian term. If the eigenvectors σ and μ have vanishing eigenvalues, it could be seen that the Laplacian term vanishes synchronously. To formulate the Laplacian term in the governing equation, eigenvectors beyond the displaced Planck distribution should be entangled with the first four eigenvectors and given non-vanishing eigenvalues. This treatment is consistent with the Chapman-Enskog expansion in Sec. IV A.

In the derivation in Sec. III, the displaced Planck distribution is adopted. If only the first two terms in Eq. (23) are considered, the distribution functions f_E and f_+ are the eigenvector with vanishing eigenvalues of the normal collision matrix by a Krumhansl's transform (see Eq. (17) in Ref. 17). However, $f_E + f_+$ is just a first order approximation of f_D. If f_1, f_2, and f_3 are strictly proportional to the heat flux, they should have small but non-vanishing eigenvalues; if they have vanishing eigenvalues, they should contain high orders of the heat flux. Neglecting such effects will drop the convective terms in Eq. (30).

V. CONCLUSION

1) A Brinkman extension is introduced into the thermomass momentum conservation equation as a Laplacian term, which is important when the characteristic size of the system is comparable with the mean free path of energy carriers. This extension introduces the viscosity of the thermomass and occurs in media only if the thermal transport behavior in the boundary layer is significant. The resultant governing equation includes the pressure gradient (driving force), inertia, and friction terms (resistant force). The extended thermomass governing equation is applicable for nanosystems in which the Knudsen number is large. This equation is consistent with the G-K model with a convection term, which is also addressed as the nonlinear G-K equation.
2) The phonon Boltzmann equations are used to deduce the governing equation with the concept of thermomass. Assuming that the real distribution could be characterized by a second order Taylor series expansion of the displaced Planck distribution, we derive the governing equation, which is close to that given by the thermomass theory. The concept of thermomass guides the process to transform the Boltzmann equation to the conservation equations of mass and momentum, just as in hydrodynamics. The driving force of heat conduction is described by the pressure gradient. However, the convective term may be not full through the Doppler effect, i.e., the change of frequency when the phonon gas is drifting.
3) Compared with the Chapman-Enskog expansion and the Eigen analysis in phonon hydrodynamics, the convective term in the present governing equation comes from a higher order approximation of the displaced Planck distribution, and the Laplacian term comes from the deviation of the real distribution from the displaced Planck distribution. The deviation is usually assumed to be proportional to the relaxation time of the normal collision, so the coefficients of the Laplacian term in the governing equation behave similarly. This behavior is similar to the derivation of the Laplacian term in Navier-Stokes equation through the Chapman-Enskog expansion in hydrodynamics.
4) It should be pointed out that this paper does not consider phonon-wall interactions, which are actually important for the theory of phonon hydrodynamics and its applications in nanosystems. The slip boundary condition of heat flow at high Knudsen number, which may play a significant role in nanoscale heat conduction, should be taken into account. We are on the way to investigate the thermomass model and phonon hydrodynamics at high Knudsen numbers.

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