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Fractional-order heat conduction models from generalized Boltzmann transport equation

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The relationship between fractional-order heat conduction models and Boltzmann transport equations (BTEs) lacks a detailed investigation. In this paper, the continuity, constitutive and governing equations of heat conduction are derived based on fractional-order phonon BTEs. The underlying microscopic regimes of the generalized Cattaneo equation are thereafter presented. The effective thermal conductivity κ_{eff} converges in the subdiffusive regime and diverges in the superdiffusive regime. A connection between the divergence and mean-square displacement $\langle|\Delta x|^2\rangle \sim t^{\gamma}$ is established, namely, $\kappa_{\text{eff}} \sim t^{\gamma-1}$, which coincides with the linear response theory. Entropic concepts, including the entropy density, entropy flux and entropy production rate, are studied likewise. Two non-trivial behaviours are observed, including the fractional-order expression of entropy flux and initial effects on the entropy production rate. In contrast with the continuous time random walk model, the results involve the non-classical continuity equations and entropic concepts.

This article is part of the theme issue 'Advanced materials modelling via fractional calculus: challenges and perspectives'.

1. Introduction

The macroscopic description of heat conduction was established by Fourier in the nineteenth century, which formulates the heat flux $\mathbf{q} = \mathbf{q}(\mathbf{x}, t)$ in terms of the local

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temperature field $T = T(\mathbf{x}, t)$, namely

$$\mathbf{q} + \kappa \nabla T = \mathbf{0}. \tag{1.1}$$

In the above equation, the coefficient κ is termed thermal conductivity, which is an intrinsic material property and should be independent of the geometrical parameters such as the system size L. One general approach to predict the thermal conductivity is based on the linearized Boltzmann transport equation (BTE) [1–3]. The following phonon BTE with the single-mode relaxation time (SMRT) approximation [3] is a typical example:

$$\frac{\partial f}{\partial t} + \mathbf{v}_\mathrm{g} \cdot \nabla f = \frac{f_0 - f}{\tau}, \tag{1.2}$$

where $f = f(\mathbf{x}, t, \mathbf{k})$ is the phonon distribution function, $\mathbf{k}$ denotes the wavevector, $\mathbf{v}_\mathrm{g}$ stands for the phonon group velocity, τ is the relaxation time, $f_0 = 1/(\exp(\hbar\omega/k_\mathrm{B}T) - 1)$ is the equilibrium distribution, $\hbar$ is the reduced Planck constant, ω is the angular frequency and k_B is the Boltzmann constant. In isotropic cases, equation (1.2) gives rise to the following prediction:

$$\kappa = \frac{1}{3} c |\mathbf{v}_\mathrm{g}| l, \tag{1.3}$$

with c the specific heat capacity per unit volume and $l = |\mathbf{v}_\mathrm{g}|\tau$ the mean free path (MFP).

Furthermore, the BTE also predicts violations of Fourier's Law when the characteristic size and time are comparable to (or even smaller than) the MFP and relaxation time of heat carriers, respectively. For instance, the equation of phonon radiative transfer (EPRT) [2] leads to a non-Fourier relation between the one-dimensional (1D) heat flux q_x and temperature difference ΔT:

$$q_x = \frac{1}{1 + (4/3)Kn} \left(\frac{1}{3} c |\mathbf{v}_\mathrm{g}| l \right) \frac{\Delta T}{L}, \tag{1.4}$$

with $Kn = l/L$ standing for the Knudsen number. The above equation implies a length-dependent effective thermal conductivity $\kappa_\mathrm{eff} = \kappa_\mathrm{eff}(L)$ in stationary problems, while non-Fourier behaviours exist in non-stationary situations as well. For non-stationary heat conduction, the SMRT approximation does not agree with Fourier's Law rigorously but leads to the Cattaneo–Vernotte (CV) model [4,5] as follows:

$$\mathbf{q} + \tau \frac{\partial \mathbf{q}}{\partial t} = -\kappa \nabla T. \tag{1.5}$$

Upon combining the above equation with the standard continuity equation,

$$\frac{\partial e}{\partial t} = c \frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{q}, \tag{1.6}$$

with $e = e(\mathbf{x}, t)$ the local energy density, one can acquire a hyperbolic governing equation for the local temperature, namely

$$\frac{\partial T}{\partial t} + \tau \frac{\partial^2 T}{\partial t^2} = D \nabla^2 T, \tag{1.7}$$

with $D = \kappa/c$ denoting the thermal diffusivity. Equation (1.7) is able to avoid the infinite speed of heat propagation traceable to the parabolic governing equation of Fourier's Law. However, it is likewise paired with some unsatisfactory features [6–10], i.e. the negative entropy production rate and absolute temperature.

In the past decades, fractional-order generalizations of equations (1.5)–(1.7) have attracted increasing interest [11–14]. Through introducing the fractional-order derivatives into the constitutive and continuity equations, Compte & Metzler [11] proposed a class of temporal fractional-order models termed generalized Cattaneo equations (GCEs). They also studied the long-time and short-time asymptotic behaviours of the mean-square displacement (MSD). Kosztołowicz & Lewandowska [12] applied the GCE class to the subdiffusive transport of electrolytes, while Povstenko [13] introduced the spatial fractional-order derivative in the theories of thermal stresses. The numerical solutions of these fractional-order generalizations have been investigated likewise [14]. Since the standard CV model can be derived from the phonon BTE, a natural question is: Can these fractional-order heat conduction models emerge from the

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phonon BTE or its generalizations? This question has not been much studied [15], and the main aim of the present work is to address it. In this work, we show that fractional-order continuity, constitutive and governing equations of heat conduction can be derived from the fractional-order phonon BTEs. The underlying microscopic regimes of these models are thereafter presented. The corresponding entropic concepts, including the entropy density, entropy flux and entropy production rate, are also discussed. Different from other fractional-order approaches, the fractional-order BTEs will give rise to several non-classical results. The present work will cover the results of Li & Cao [15], but be more strict and complete in three aspects. First, the initial value terms will be considered, which are neglected in [15]. Second, Li & Cao [15] only discuss the entropic concepts for the Goychuk's model, while this work will study other fractional-order BTEs as well. Third, Li & Cao [15] do not distinguish the phonon relaxation time and dimension parameter, which will be discussed in this work.

2. Constitutive and continuity equations

We first recall the relation between the distribution function and macroscopic thermodynamic quantities. The local phonon energy density is given by

$$e = \int f\hbar\omega \, \mathrm{d}\mathbf{k} = \int f_0\hbar\omega \, \mathrm{d}\mathbf{k}, \tag{2.1}$$

while the heat flux is written as

$$\mathbf{q} = \int \mathbf{v}_\mathrm{g} f\hbar\omega \, \mathrm{d}\mathbf{k} = \int \mathbf{v}_\mathrm{g}(f - f_0)\hbar\omega \, \mathrm{d}\mathbf{k}. \tag{2.2}$$

In the spirit of Nonnenmacher & Nonnenmacher [16], equation (1.2) can be generalized into the following fractional-order form:

$$\frac{\partial f}{\partial t} + \tau_\alpha^{1-\alpha} D_t^{1-\alpha}(\mathbf{v}_\mathrm{g} \cdot \nabla f) = \tau_\alpha^{1-\alpha} D_t^{1-\alpha}\left(\frac{f_0 - f}{\tau}\right), \tag{2.3}$$

where $\alpha \in (0, 1)$ and $\tau_\alpha > 0$ is a constant parameter of dimension second. The temporal fractional-order derivative $D_t^{1-\alpha}$ is usually selected as the Riemann–Liouville (RL) operator on the right-hand side:

$$D_t^{1-\alpha} = {}_0^{\mathrm{RL}}D_t^{1-\alpha} f(\mathbf{x}, t, \mathbf{k}) = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{f(\mathbf{x}, t', \mathbf{k})}{|t - t'|^{1-\alpha}} \, \mathrm{d}t'. \tag{2.4}$$

Upon multiplying equation (2.3) by $\hbar\omega$ and integrating it over the wavevector space, we obtain

$$\begin{aligned} \frac{\partial e}{\partial t} = c\frac{\partial T}{\partial t} &= \int \frac{\partial f}{\partial t}\hbar\omega \, \mathrm{d}\mathbf{k} \\ &= -\nabla \cdot \int (\tau_\alpha^{\alpha-1} D_t^{1-\alpha} \mathbf{v}_\mathrm{g} f)\hbar\omega \, \mathrm{d}\mathbf{k} \\ &= -\tau_\alpha^{1-\alpha} D_t^{1-\alpha}(\nabla \cdot \mathbf{q}), \end{aligned} \tag{2.5}$$

which deviates from the standard continuity equation. Substituting equation (2.3) into $\tau_\alpha^{1-\alpha} D_t^{1-\alpha}\mathbf{q}/\tau$ yields

$$\begin{aligned} \frac{\tau_\alpha^{1-\alpha} D_t^{1-\alpha}\mathbf{q}}{\tau} &= \int \mathbf{v}_\mathrm{g} \tau_\alpha^{1-\alpha} D_t^{1-\alpha}\left(\frac{f - f_0}{\tau}\right)\hbar\omega \, \mathrm{d}\mathbf{k} \\ &= -\int \mathbf{v}_\mathrm{g}\left[\frac{\partial f}{\partial t} + \tau_\alpha^{1-\alpha} D_t^{1-\alpha}(\mathbf{v}_\mathrm{g} \cdot \nabla f)\right]\hbar\omega \, \mathrm{d}\mathbf{k} \\ &= -\frac{\partial}{\partial t}\left(\int \mathbf{v}_\mathrm{g} f\hbar\omega \, \mathrm{d}\mathbf{k}\right) - \tau_\alpha^{1-\alpha} D_t^{1-\alpha}\left(\int \mathbf{v}_\mathrm{g}\mathbf{v}_\mathrm{g} \cdot \nabla f\hbar\omega \, \mathrm{d}\mathbf{k}\right) \\ &= -\frac{\partial \mathbf{q}}{\partial t} - \tau_\alpha^{1-\alpha} D_t^{1-\alpha}\int \mathbf{v}_\mathrm{g}\mathbf{v}_\mathrm{g}\nabla f\hbar\omega \, \mathrm{d}\mathbf{k}. \end{aligned} \tag{2.6}$$

In order to establish a relationship between the heat flux and temperature distribution, we shall assume local equilibrium, $\nabla f \cong \nabla f_0$. Equation (2.6) therefore becomes

$$\tau \frac{\partial \mathbf{q}}{\partial t} + \tau_\alpha^{1-\alpha} D_t^{1-\alpha} \mathbf{q} = -\tau_\alpha^{1-\alpha} D_t^{1-\alpha} (\kappa \nabla T), \tag{2.7}$$

which reduces to the CV model as $\alpha = 1$. We now focus on the governing equation of the local temperature. Taking an integral $\tau_\alpha^{\alpha-1} D_t^{\alpha-1}$ in equation (2.5) leads to

$$\tau_\alpha^{\alpha-1} D_t^{\alpha-1} \left(c \frac{\partial T}{\partial t} \right) = -\nabla \cdot \mathbf{q} + \frac{1}{t^\alpha \Gamma(1-\alpha)} [D_t^{-\alpha} (\nabla \cdot \mathbf{q})]|_{t=0}, \tag{2.8}$$

while the divergence of equation (2.7) reads

$$\tau \frac{\partial}{\partial t} (\nabla \cdot \mathbf{q}) + \tau_\alpha^{1-\alpha} D_t^{1-\alpha} (\nabla \cdot \mathbf{q}) = -\tau_\alpha^{1-\alpha} D_t^{1-\alpha} (\kappa \nabla^2 T). \tag{2.9}$$

Upon substituting equation (2.8) into equation (2.9), we can derive

$$\begin{aligned} &\tau \tau_\alpha^{\alpha-1} \left(D_t^{\alpha+1} T + \frac{T|_{t=0}}{t^{\alpha+1} \Gamma(1-\alpha)} \right) + \frac{\alpha \tau [D_t^{-\alpha} (\nabla \cdot \mathbf{q})]|_{t=0}}{t^{\alpha+1} c \Gamma(1-\alpha)} + \frac{\partial T}{\partial t} - \frac{[D_t^{-\alpha} (\nabla \cdot \mathbf{q})]|_{t=0}}{c t \tau_\alpha^{\alpha-1}} \\ &= \tau_\alpha^{1-\alpha} D_t^{1-\alpha} (D \nabla^2 T). \end{aligned} \tag{2.10}$$

Different from the integer-order models, equation (2.10) contains several initial value terms. In the short-time limit $t \to 0$, these initial value terms will cause singularities. In the long-time limit $t \to +\infty$, these initial value terms tend to zero. If the initial value terms are neglected, it becomes

$$\tau \tau_\alpha^{\alpha-1} D_t^{\alpha+1} T + \frac{\partial T}{\partial t} = \tau_\alpha^{1-\alpha} D_t^{1-\alpha} (D \nabla^2 T), \tag{2.11}$$

which can be reformulated as

$$\tau \tau_\alpha^{2\alpha-2} D_t^{2\alpha} T + \tau_\alpha^{\alpha-1} D_t^\alpha T = D \nabla^2 T. \tag{2.12}$$

The above equation belongs to the GCE class if $\tau = \tau_\alpha$, and, more precisely, it is nothing but the GCE I [11]. It should be mentioned that the relaxation time τ and parameter τ_α possess fundamentally different physical meanings: τ_α is paired with the fractional-order derivative, which is necessary to guarantee the physical dimension; τ reflects the phonon scattering, and, in more refined descriptions, it will depend on the angular frequency and wavevector, namely, $\tau = \tau(\mathbf{k}, \omega)$. Hence, it is not appropriate to equate τ to τ_α.

Note that in the work by Compte & Metzler [11], the GCE I arises from the following continuity and constitutive equations, respectively:

$$c \tau_\alpha^\alpha D_t^\alpha T = -\nabla \cdot \mathbf{q} \tag{2.13}$$

and

$$\mathbf{q} + \tau_\alpha^\alpha D_t^\alpha \mathbf{q} = -\kappa \nabla T. \tag{2.14}$$

The above equations will equal equations (2.5) and (2.7), respectively, when the initial value terms are neglected. In the presence of the initial value terms, a strict derivation of equations (2.13) and (2.14) should be based on the following BTE:

$$\tau_\alpha^{\alpha-1} D_t^\alpha f + \mathbf{v}_g \cdot \nabla f = \frac{f_0 - f}{\tau}. \tag{2.15}$$

Although both equations (2.3) and (2.15) can lead to the GCE I, their differences cannot be ignored. There is no stationary solution for equation (2.15) because $\tau_\alpha^{\alpha-1} D_t^\alpha f$ remains time-dependent even if f is time-independent. The same problem also occurs in equation (2.14). It indicates that stationary heat transport does not exist for equations (2.15) and (2.14), which is unsatisfactory. By contrast, a time-independent distribution function is able to fulfil equation (2.3) if it satisfies

$$\mathbf{v}_g \cdot \nabla f = \frac{f_0 - f}{\tau}. \tag{2.16}$$

This shows that equation (2.3) is equivalent to the standard BTE for stationary heat transport. Accordingly, we suggest equation (2.3) rather than equation (2.15) as the BTE for the GCE I. Correspondingly, equations (2.5) and (2.7) are better choices for the continuity and constitutive equations than equations (2.13) and (2.14). In the limit $\tau_\alpha \to 0$, equation (2.3) allows any time-independent distribution functions, whereas the solution of equation (2.15) must satisfy equation (2.16).

We now consider another fractional-order form given by Goychuk [17]:

$$\frac{\partial f}{\partial t} + \mathbf{v}_g \cdot \nabla f = \tau_\alpha^{1-\alpha} D_t^{1-\alpha}\left(\frac{f_0 - f}{\tau}\right). \tag{2.17}$$

Using a similar derivation, one can find that the standard continuity equation is recovered, while the constitutive relation is written as

$$\tau \frac{\partial \mathbf{q}}{\partial t} + \tau_\alpha^{1-\alpha} D_t^{1-\alpha} \mathbf{q} = -\kappa \nabla T. \tag{2.18}$$

Combining the continuity and constitutive equations yields

$$\tau_\alpha^{1-\alpha} D_t^{2-\alpha} T + \tau \frac{\partial^2 T}{\partial t^2} = D \nabla^2 T + \frac{T|_{t=0}\tau_\alpha^{1-\alpha}}{t^{2-\alpha}\Gamma(\alpha - 1)}, \tag{2.19}$$

which agrees with the GCE II with the initial value term neglected. In [11], the GCE II is a result of the standard continuity equation and the following constitutive equation:

$$\mathbf{q} + \tau \tau_\alpha^{\alpha-1} D_t^{\alpha} \mathbf{q} = -\tau_\alpha^{\alpha-1} D_t^{\alpha-1}(\kappa \nabla T). \tag{2.20}$$

The above equation can be derived from the following BTE:

$$\tau_\alpha^{\alpha-1} D_t^{\alpha} f + \tau_\alpha^{\alpha-1} D_t^{\alpha-1}(\mathbf{v}_g \cdot \nabla f) = \frac{f_0 - f}{\tau}. \tag{2.21}$$

However, the above equation cannot recover the standard continuity equation rigorously. Upon multiplying equation (2.21) by $\hbar\omega$ and integrating it over the wavevector space, we arrive at

$$\begin{aligned} &\int [\tau_\alpha^{\alpha-1} D_t^{\alpha} f + \tau_\alpha^{\alpha-1} D_t^{\alpha-1}(\mathbf{v}_g \cdot \nabla f)]\hbar\omega\, \mathrm{d}\mathbf{k} \\ &\quad = \int \left[\tau_\alpha^{\alpha-1} D_t^{\alpha-1}\left(\frac{\partial f}{\partial t} + \mathbf{v}_g \cdot \nabla f\right) + \frac{f|_{t=0}}{t^{\alpha}\Gamma(1-\alpha)}\right]\hbar\omega\, \mathrm{d}\mathbf{k} \\ &\quad = \tau_\alpha^{\alpha-1} D_t^{\alpha-1}\left(\frac{\partial e}{\partial t} + \nabla \cdot \mathbf{q}\right) + \frac{e|_{t=0}}{t^{\alpha}\Gamma(1-\alpha)}. \end{aligned} \tag{2.22}$$

From equation (2.22), we can find that the standard continuity equation no longer holds unless $e|_{t=0} = 0$. Accordingly, we suggest equation (2.17) rather than equation (2.21) as the BTE for the GCE II.

The last case is that the temporal fractional-order derivative only appears in the drift term, namely

$$\frac{\partial f}{\partial t} + \tau_\alpha^{1-\alpha} D_t^{1-\alpha}(\mathbf{v}_g \cdot \nabla f) = \frac{f_0 - f}{\tau}. \tag{2.23}$$

This fractional-order BTE will give rise to the same continuity equation as equation (2.5), while the constitutive equation takes the following form:

$$\tau \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -\tau_\alpha^{1-\alpha} D_t^{1-\alpha}(\kappa \nabla T). \tag{2.24}$$

The corresponding governing equation is given by

$$\tau_\alpha^{\alpha-1}\left[D_t^\alpha T + \tau D_t^{\alpha+1} T + \frac{(\tau+t)T|_{t=0}}{t^{\alpha+1}\Gamma(1-\alpha)}\right] + \frac{\alpha\tau[D_t^{-\alpha}(\nabla\cdot\mathbf{q})]|_{t=0}}{t^{\alpha+1}c\Gamma(1-\alpha)} - \frac{[D_t^{-\alpha}(\nabla\cdot\mathbf{q})]|_{t=0}}{t^{\alpha}c\Gamma(1-\alpha)}$$
$$= \tau_\alpha^{1-\alpha} D_t^{1-\alpha}(D\nabla^2 T). \quad (2.25)$$

In the absence of the initial value terms, equation (2.25) can be transformed into the GCE III. In [11], the GCE III arises from the standard CV model and equation (2.13). The standard CV model should correspond to the standard BTE, which likewise gives rise to the standard continuity equation. Thus, the derivation in [11] is invalid in phonon heat transport, and we suggest equations (2.5) and (2.24) as the continuity and constitutive equations for the GCE III. The foundation of the above generalized BTEs can be related to the fractional variational principles [18].

3. Discussion on non-Brownian exponent

The GCE class describes anomalous diffusion, which is characterized by the long-time asymptotics of the MSD, $\langle|\Delta x|^2\rangle \sim t^\gamma$. The range of the non-Brownian exponent γ is commonly classified into five subranges: hyperdiffusion, $\gamma > 2$; ballistic motion, $\gamma = 2$; superdiffusion, $1 < \gamma < 2$; normal diffusion, $\gamma = 1$; and subdiffusion, $0 < \gamma < 1$. According to the result by Compte & Metzler [11], $\gamma = \alpha \in (0, 1)$ for the GCEs I and III, while for the GCE II, $\gamma = 2 - \alpha \in (1, 2)$. It indicates that the GCEs I and III correspond to subdiffusive heat conduction, while the GCE II is for superdiffusive heat conduction. For the two constitutive equations of the GCE I, equations (2.3) and (2.14), a time-independent temperature distribution will give rise to a convergent heat flux as $t \to +\infty$, which is true for the GCE III as well. In contrast to the GCEs I and III, the two constitutive equations for the GCE II, equations (2.18) and (2.20), predict a power-law divergence $\mathbf{q} \sim t^{1-\alpha}$ as $t \to +\infty$. These results imply convergent effective thermal conductivity in the subdiffusive regime and divergent effective thermal conductivity in the superdiffusive regime, which is consistent with existing understandings of anomalous heat diffusion [19–22]. Specifically, there is a connection between the divergence and non-Brownian exponent, namely

$$\mathbf{q} \sim t^{1-\alpha} = t^{\gamma-1} \quad \Rightarrow \quad \kappa_{\mathrm{eff}} \sim t^{\gamma-1}. \quad (3.1)$$

The above equation has been demonstrated in the framework of the linear response theory [19], which is likewise supported by numerical calculations [23–27]. In the short-time limit $t \to 0$, singularities will occur in the initial value terms, which can be eliminated via replacing the RL operator with other non-singular derivatives [28,29]. It should be mentioned that we here neglect the anomalies traceable to the standard case with $\alpha = 1$, which has been widely discussed in existing investigations [30–34].

4. Entropic concepts

In this section, we will investigate three entropic concepts based on the above BTEs, including the entropy density $s = s(\mathbf{x}, t)$, entropy flux $\mathbf{J} = \mathbf{J}(\mathbf{x}, t)$ and entropy production rate $\sigma = \sigma(\mathbf{x}, t)$. We mention that there exists careful discussion [35] on the entropic definitions in fractional-order heat conduction, yet the underlying microscopic regimes have not been investigated. The relation of these entropic concepts is expressed by the entropy balance equation as follows:

$$\frac{\partial s}{\partial t} = -\nabla \cdot \mathbf{J} + \sigma. \quad (4.1)$$

In phonon heat transport, the entropy density is formulated as

$$s = k_{\mathrm{B}} \int [(f+1)\ln(f+1) - f\ln f]\,\mathrm{d}\mathbf{k}, \quad (4.2)$$

whose derivative is given by

$$\frac{\partial s}{\partial t} = k_B \int \frac{\partial f}{\partial t}[\ln(f+1) - \ln f]\,d\mathbf{k}. \tag{4.3}$$

In the near-equilibrium region, $|f - f_0| = o(f_0)$, the entropy density coincides with the classical irreversible thermodynamics [36]:

$$\begin{aligned}\frac{\partial s}{\partial T} &= k_B \int \frac{\partial f}{\partial T} \ln\frac{f+1}{f}\,d\mathbf{k} \\ &\approx k_B \int \frac{\partial f_0}{\partial T} \ln\frac{f_0+1}{f_0}\,d\mathbf{k} = k_B \int \frac{\partial f_0}{\partial T}\frac{\hbar\omega}{k_B T}\,d\mathbf{k} \\ &= \frac{1}{T}\int \frac{\partial f_0}{\partial T}\hbar\omega\,d\mathbf{k} = \frac{c}{T} \quad \Rightarrow \quad s = \int \frac{c\,dT}{T}.\end{aligned} \tag{4.4}$$

Through substituting equation (2.3) into equation (4.3), we can obtain

$$\frac{\partial s}{\partial t} = k_B \int \left(\ln\frac{f+1}{f}\right) \tau_\alpha^{1-\alpha} D_t^{1-\alpha} \left(\frac{f_0 - f}{\tau} - \mathbf{v}_g \cdot \nabla f\right) d\mathbf{k}. \tag{4.5}$$

In the standard case, the term containing $(f_0 - f)/\tau$ corresponds to the entropy production rate, while the term containing $(\mathbf{v}_g \cdot \nabla f)$ emerges from the entropy flux. Therefore, we have

$$\nabla \cdot \mathbf{J} = k_B \int \left(\ln\frac{f+1}{f}\right) \tau_\alpha^{1-\alpha} D_t^{1-\alpha} (\mathbf{v}_g \cdot \nabla f)\,d\mathbf{k} \tag{4.6}$$

and

$$\sigma = k_B \int \left(\ln\frac{f+1}{f}\right) \tau_\alpha^{1-\alpha} D_t^{1-\alpha} \left(\frac{f_0 - f}{\tau}\right) d\mathbf{k}. \tag{4.7}$$

Specifically, equation (4.6) can be simplified as an explicit form if $\alpha = 1$, namely

$$\mathbf{J} = k_B \int \mathbf{v}_g[(f+1)\ln(f+1) - f\ln f]\,d\mathbf{k}. \tag{4.8}$$

We now approximate the entropy flux and entropy production rate in the near-equilibrium region. Using the approximation $\ln f + 1/f \approx \ln f_0 + 1/f_0 = \hbar\omega/k_B T$ in equation (4.6), we obtain

$$\begin{aligned}\nabla \cdot \mathbf{J} &\approx k_B \int \frac{\hbar\omega}{k_B T} \tau_\alpha^{1-\alpha} D_t^{1-\alpha} (\mathbf{v}_g \cdot \nabla f)\,d\mathbf{k} \\ &= \frac{1}{T}\tau_\alpha^{1-\alpha} D_t^{1-\alpha}\left[\nabla \cdot \left(\int \mathbf{v}_g f \hbar\omega\,d\mathbf{k}\right)\right] = \frac{1}{T}\tau_\alpha^{1-\alpha} D_t^{1-\alpha}(\nabla \cdot \mathbf{q}),\end{aligned} \tag{4.9}$$

and substituting equation (4.9) into equation (4.1) leads to $\sigma \approx 0$. It means that σ is a higher-order small quantity of $o(|f - f_0|)$. For equation (2.15), equation (4.6) is still valid, while the entropy production rate is given by

$$\sigma = k_B \int \ln\frac{f+1}{f}\left[\tau_\alpha^{1-\alpha} D_t^{1-\alpha}\left(\frac{f_0 - f}{\tau}\right) + \frac{(D_t^{\alpha-1} f)|_{t=0}}{\Gamma(\alpha - 1)t^{2-\alpha}}\right] d\mathbf{k}. \tag{4.10}$$

Equation (4.10) shows that the initial effects will also contribute to the entropy production rate. The macroscopic approximation of the entropy flux remains (4.9), yet the entropy production rate is approximated by

$$\sigma \approx \frac{(D_t^{\alpha-1} e)|_{t=0}}{T\Gamma(\alpha - 1)t^{2-\alpha}} > 0. \tag{4.11}$$

For equation (2.17), the entropy flux is equation (4.8), while the entropy production reads

$$\sigma = k_B \int \ln\frac{f+1}{f}\left(\frac{f_0 - f}{\tau}\right) d\mathbf{k}. \tag{4.12}$$

The corresponding first-order approximations coincide with classical irreversible thermodynamics, namely

$$\mathbf{J} \approx \frac{\mathbf{q}}{T} \tag{4.13}$$

and

$$\sigma \approx \mathbf{q} \cdot \nabla \left(\frac{1}{T} \right). \tag{4.14}$$

For equation (2.21), the entropy flux obeys equation (4.8), and the entropy production rate is given by equation (4.10). Correspondingly, the entropy flux and entropy production rate are approximated by equations (4.12) and (4.11), respectively. For equation (2.23), equations (4.6) and (4.12) still hold, while the macroscopic approximations are the same as the approximations for equation (2.3).

5. Conclusion

Fractional-order continuity and constitutive equations of heat conduction are derived based on fractional-order phonon BTEs. The fractional-order governing equations are then established, and in the absence of the initial value terms, these governing equations will agree with the GCE class. The underlying microscopic regimes of these models are thereafter presented, namely, the memory effects in phonon transport.

The effective thermal conductivity converges in the subdiffusive regime and diverges in the superdiffusive regime, which agrees with existing understandings of anomalous heat diffusion. A connection between the divergence and non-Brownian exponent is observed, namely, $\kappa_{\text{eff}} \sim t^{\gamma-1}$, which is consistent with the linear response theory. Such power-law divergences have been widely observed in low-dimensional systems [24–27], and hence our models can be applied to heat conduction in low-dimensional systems like one-dimensional momentum-conserving lattices [26].

Three entropic concepts, i.e. the entropy density, entropy flux and entropy production rate, are studied based on the fractional-order BTEs. Two non-trivial behaviours are found, namely, the fractional-order relationship between the heat flux and entropy flux, and the initial effects on the entropy production rate.

Compared with Denisov *et al.* [21], wherein the heat carriers are particles obeying the continuous-time random walk model, this work focuses on heat conduction dominated by phonons. In this work, the constitutive, continuity and governing equations are derived from the fractional-order BTEs. However, Denisov *et al.* [21] assume the standard continuity equation, and there is no rigorous constitutive relation between the heat flux and temperature distribution. Furthermore, this work illustrates that the entropic concepts can deviate from the classical formula, which is the basis of [21].

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