



Anomalous heat diffusion from fractional Fokker–Planck equation

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ABSTRACT

Anomalous heat diffusion, which is commonly characterized by the nonlinear growth of mean square of displacement (MSD), $\langle |\Delta x|^2 \rangle \sim t^\beta$ ($0 < \beta \leq 2$), is usually paired with a length-dependence of effective thermal conductivity κ_{eff} , namely, $\kappa_{eff} \sim L^\alpha$ with L the system length. In this work, a generic time- and length-dependence of κ_{eff} is obtained based on the fractional Fokker–Planck equation (FFPE) with orders $(\gamma, \mu) \in \mathbb{R}^2$, namely, $\kappa_{eff} \propto t^{\gamma-1} L^{-\mu}$. Two existing paradigmatic results, $\kappa_{eff} \propto t^{\beta-1}$ and $\kappa_{eff} \propto L^{2-2/\beta}$, are first unified in our work, which reflect memory effects and nonlocality in energy fluctuations, respectively. We formulate the effective thermal conductivity in terms of entropy generation, which does not rely on the local-equilibrium hypothesis.

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1. Introduction

Classical Fourier's law of heat conduction,

$$\mathbf{q} = -\kappa \nabla T, \quad (1.1)$$

where $\mathbf{q} = \mathbf{q}(\mathbf{x}, t)$ is the local heat flux density, κ is the thermal conductivity and $T = T(\mathbf{x}, t)$ is the local temperature, has been proved by numerous experiments in three-dimensional (3D) bulk materials. However, its validity is debatable in one-dimensional (1D) and quasi-one-dimensional systems [1,2]. In such cases, there is no well-defined thermal conductivity and the effective thermal conductivity κ_{eff} becomes length-dependent. The power-law length-dependence, namely, $\kappa_{eff} \sim L^\alpha$ with L the system length, is commonly observed, i.e., 1D momentum-conserving systems [3] and the Fermi–Pasta–Ulam (FPU) model [2]. Positive α will give rise to a sharp enhancement of heat transport with increasing lengths, which is intriguing in engineering. In a recent experimental investigation by Lee et al. [4], the power-law exponent is reported as $0.1 \leq \alpha \leq 0.5$. Similar non-universal anomaly was also observed in numerical calculation [5].

One universal approach for predicting α is through anomalous heat diffusion [6–11], which is commonly characterized by the nonlinear growth of the mean square of displacement (MSD) [12], $\langle |\Delta x|^2 \rangle \sim t^\beta$ ($0 < \beta \leq 2$). Based on the Lévy-walk (LW) model of anomalous diffusion, Denisov et al. [6] have established

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$\alpha = \beta - 1$. This relation is also derived in the framework of the linear response theory [7], which does not assume any specific random walk model. Relying on the length-dependence of the mean first passage time (MFPT), Li and Wang [8] acquired a different result, $\alpha = 2 - 2/\beta$. There are two different relations, and whether they can be unified in one generic model remains an open problem. In the following, we will address this problem based on Fokker–Planck dynamics.

The connection between Fokker–Planck dynamics and heat conduction arises from the governing equation of Fourier’s law, namely,

$$\mathcal{L}_{FP}[T] = \frac{\partial T}{\partial t} - D \nabla^2 T = 0, \quad (1.2)$$

where $D = \kappa/c$ denotes the thermal diffusivity and c is the specific heat capacity per volume. If T is replaced by the probability distribution function (PDF) $P = P(\mathbf{x}, t)$, it becomes the standard Fokker–Planck equation (FPE) in the absence of an external force field, which describes normal diffusion. Proceeding from this, the FPE approach, which formulates the continuous-time random walk (CTRW), has been applied to Fourier and non-Fourier heat conduction. In Dhar’s review article [1], the correlation function of energy fluctuations $C_{ee} = C_{ee}(\mathbf{x}, t)$ is assumed to satisfy $\mathcal{L}_{FP}[C_{ee}] = 0$, which is used to derive the Green–Kubo formula. The PDF can be defined as the normalization of C_{ee} , and one can obtain $\mathcal{L}_{FP}[P] = 0$ from Dhar’s model. Razi-Naqvi and Waldenström [13] considered a non-Markovian FPE for the evolution of $T(\mathbf{x}, t)$ in phonon heat transport, which avoids the artificial wave front in the hyperbolic governing equation [14,15]. Nevertheless, generalized FPEs for anomalous diffusion such as fractional derivatives [16–25], are not much involved. In the present work, 1D anomalous heat diffusion is investigated by the fractional Fokker–Planck equation (FFPE) as follows

$$\frac{\partial P}{\partial t} = D_t^{1-\gamma} \left[K_{(\gamma, \mu)} \frac{\partial^{\mu+2} P}{\partial x^{\mu+2}} \right], \quad (1.3)$$

where the orders $(\gamma, \mu) \in \mathbb{R}^2$ and $K_{(\gamma, \mu)}$ is a generalized diffusion coefficient. Eq. (1.3) can be understood as a non-Brownian generalization of Dhar’s model, whose long-time asymptotics of the MSD obeys $\beta = 2\gamma/(\mu + 2)$. In the following, we will show $\kappa_{eff} \propto t^{\gamma-1} L^{-\mu}$, which expects the two scaling laws, $\alpha = \beta - 1$ and $\alpha = 2 - 2/\beta$, in two special cases respectively.

2. Temporal fractional-order case

Eq. (1.3) can be regarded as a result of the continuity equation

$$\frac{\partial P}{\partial t} + \frac{\partial J}{\partial x} = 0, \quad (2.1)$$

and a fractional-order constitutive equation for the probability current $J = J(x, t)$:

$$J = -K_{(\gamma, \mu)} D_t^{1-\gamma} \frac{\partial^{\mu+1} P}{\partial x^{\mu+1}}. \quad (2.2)$$

In order to use this constitutive equation in heat conduction, we consider entropy transport and production based on statistical mechanics. The entropy of a region Π is written as $S = k_B \int_{\Pi} -P \ln P$ with k_B the Boltzmann constant. One can thereafter formulate the local entropy density as $s = s[P] = -k_B P \ln P$. The time derivative of s is written as

$$\begin{aligned} \frac{\partial s}{\partial t} &= -k_B (\ln P + 1) \frac{\partial P}{\partial t} = k_B (\ln P + 1) \frac{\partial P}{\partial x} \\ &= \frac{\partial}{\partial x} [k_B \mathbf{J} (\ln P + 1)] - k_B J \frac{\partial}{\partial x} (\ln P). \end{aligned} \quad (2.3)$$

The term $\sigma = -k_B J \frac{\partial}{\partial x} (\ln P)$ usually corresponds to the entropy production rate, and the entropy flux $j = j(x, t)$ can be obtained from the following entropy balance equation

$$\frac{\partial s}{\partial t} = -\frac{\partial j}{\partial x} + \sigma, \quad (2.4)$$

which leads to

$$j = -k_B J (\ln P + 1) = k_B (\ln P + 1) K_{(\gamma, \mu)} D_t^{1-\gamma} \frac{\partial^{\mu+1} P}{\partial x^{\mu+1}}. \quad (2.5)$$

In normal diffusion, $(\gamma, \mu) = (1, 0)$, Eq. (2.5) characterizes entropy transport driven by the entropy gradient, $j = -K_{(1,0)} \frac{\partial s}{\partial x}$. When $(\gamma, \mu) = (\gamma, 0)$, a stationary or quasi-stationary P will give rise to the same scheme, namely,

$$j(x, t) = -K_{(\gamma, 0)} D_t^{1-\gamma} \left[\frac{\partial s(x)}{\partial x} \right]. \quad (2.6)$$

In the near equilibrium case, $j(x, t)$ and $s(x, t)$ can be approximated as follows [26], respectively,

$$s(x, t) \cong \int^{T(x, t)} c \frac{dT}{T}, \quad (2.7)$$

$$j(x, t) \cong \frac{q(x, t)}{T(x, t)} \quad (2.8)$$

Combining the above approximations with Eq. (2.6) yields

$$q(x, t) = -K_{(\gamma, 0)} c D_t^{1-\gamma} \left[\frac{\partial T(x)}{\partial x} \right]. \quad (2.9)$$

There are various mathematical definitions for a fractional-order operator D_χ^μ , and we here consider two commonly used types, the Riemann–Liouville (RL) operator:

$$D_\chi^\mu f(., \chi) = {}^{RL}D_\chi^\mu f(., \chi) = \begin{cases} \frac{1}{\Gamma(n-\mu)} \frac{\partial^n}{\partial \chi^n} \int_0^\chi \frac{f(., \chi')}{|\chi - \chi'|^{\mu+1-n}} d\chi', \mu > 0 \\ \frac{1}{\Gamma(-\mu)} \int_0^\chi \frac{1}{|\chi - \chi'|^{\mu+1}} f(., \chi') d\chi', \mu < 0 \end{cases}, \quad (2.10)$$

and the Caputo operator:

$$D_\chi^\mu f(., \chi) = {}^CD_\chi^\mu f(., \chi) = \begin{cases} \frac{1}{\Gamma(n-\mu)} \int_0^\chi \frac{1}{|\chi - \chi'|^{\mu+1-n}} \frac{\partial^n f(., \chi')}{\partial \chi'^n} d\chi', \mu > 0 \\ \frac{1}{\Gamma(-\mu)} \int_0^\chi \frac{1}{|\chi - \chi'|^{\mu+1}} f(., \chi') d\chi', \mu < 0 \end{cases}, \quad (2.11)$$

where $n \in \mathbb{N} \cap (\mu, \mu + 1)$, $\mu \notin \mathbb{N}$, and the function $f(., \chi)$ is at least n -order differentiable. When $D_t^{1-\gamma} = {}^{RL}D_t^{1-\gamma}$, Eq. (2.9) becomes

$$q(x, t) = -\frac{K_{(\gamma, 0)} c t^{\gamma-1}}{\Gamma(\gamma)} \left[\frac{\partial T(x)}{\partial x} \right], \quad (2.12)$$

and we arrive at a time-dependent effective thermal conductivity, namely,

$$\kappa_{eff} \propto t^{\gamma-1} = t^{\beta-1} \propto \frac{d \langle |\Delta x|^2 \rangle}{dt}, \quad (2.13)$$

which agrees with Ref. [6]. For superdiffusion, $\gamma < 1$ and Eq. (2.13) is also true for the Caputo operator. The subdiffusive regime with $\gamma > 1$ indicates negative α , which implies that heat exchange tends to stop. For the Caputo operator, the subdiffusive heat flux is identically zero, which even exhibits complete “thermal insulation” in subdiffusive heat diffusion. Therefore, the Caputo operator is inapplicable to subdiffusive heat conduction.

Eq. (2.12) has been derived from the energy fluctuation in near-equilibrium situations likewise, where the non-equilibrium heat flux is expressed in terms of the equilibrium autocorrelation function. In this formalism,

a cut-off time t_C is typically introduced, $(\kappa_{eff}|_{t=t_C}) \propto t_C^{\beta-1}$. t_C is often estimated as $t_C \sim L/v_s$ with v_s the sound velocity. Then, one can acquire the power-law length-dependence $\alpha = \beta - 1$ from the temporal FFPE with the RL operator, while for the Caputo operator, $\alpha = \beta - 1$ only holds in superdiffusive heat conduction. The RL derivative describes memory of the heat carriers that $j(x, t)$ is expressed in terms of the integrated history of P in a time period $[0, t]$. Note that Eq. (2.9) relies on time-independent T . If it is extended into the case of time-dependent T , a fractional heat conduction equation (FHCE) [27] occurs,

$$\frac{\partial T}{\partial t} = K_{(\gamma,0)} D_t^{1-\gamma} (\nabla^2 T). \quad (2.14)$$

Eq. (2.14) is a direct generalization of Fourier heat conduction equation, while there likewise exist fractional-order extensions for the Cattaneo equation [28–31]. The above FHCE is not equivalent to the temporal FFPE despite the same form, which can be shown by their series expansions. For the temporal FFPE, the series expansion of Eq. (2.5) is given by

$$j = -K_{(\gamma,0)} {}^{RL}D_t^{1-\gamma} \left(\frac{\partial s}{\partial x} \right) - k_B K_{(\gamma,0)} \sum_{i=1}^{+\infty} \frac{(-1)^i}{i!} \frac{\Gamma(i+\gamma-1)}{\Gamma(\gamma-1)} \frac{\partial^i (\ln P)}{\partial t^i} {}^{RL}D_t^{1-\gamma-i} \left(\frac{\partial P}{\partial x} \right), \quad (2.15)$$

while the FHCE corresponds to

$$j = -K_{(\gamma,0)} {}^{RL}D_t^{1-\gamma} \left(\frac{\partial s}{\partial x} \right) + K_{(\gamma,0)} c \sum_{i=1}^{+\infty} \frac{(-1)^i}{i!} \frac{\Gamma(i+\gamma-1)}{\Gamma(\gamma-1)} \frac{\partial^i}{\partial t^i} \left(\frac{1}{T} \right) {}^{RL}D_t^{1-\gamma-i} \left(\frac{\partial T}{\partial x} \right). \quad (2.16)$$

Eqs. (2.15) and (2.16) have equivalent zero-order terms, but deviate from the other due to the existence of the higher-order terms. It indicates that the PDF cannot be replaced by the local temperature in the FFPE.

3. Spatial fractional-order case

We now focus on the case $(\gamma, \mu) = (1, \mu)$. The range of μ is classified into the following subranges: ballistic motion, $\mu = -1$; superdiffusion, $-1 < \mu < 0$; normal diffusion, $\mu = 0$; and subdiffusion, $\mu > 0$. Here, the system is in contact with two heat baths at $x = 0$ and $x = L$, whose temperatures $T|_{x=0,L}$ are time-independent. Without loss of generality, we set $T|_{x=0} - T|_{x=L} = \Delta T > 0$. If the RL or Caputo operator is selected, the FFPE reflects a nonlocality for $\mu \notin \mathbb{N}$, namely that the current at x depends on the global distribution in $[0, x]$. Obviously, this nonlocality is asymmetrical because the distribution in $(x, L]$ has no contribution. To reflect an isotropic nonlocality, the Caputo derivative can be naturally symmetrized as follows

$${}_0^L D_x^\mu f(\cdot, \chi) = \begin{cases} \frac{1}{2\Gamma(n-\mu)} \int_0^L \frac{1}{|\chi - \chi'|^{\mu+1-n}} \frac{\partial^n f(\cdot, \chi)}{\partial \chi'^n} d\chi', \mu > 0 \\ \frac{1}{2\Gamma(-\mu)} \int_0^L \frac{1}{|\chi - \chi'|^{\mu+1}} f(\cdot, \chi) d\chi', \mu < 0 \end{cases}. \quad (3.1)$$

When $\mu \neq 0$, the right-hand side of Eq. (3.1) is not a derivative of the local entropy, and the approach for $(\gamma, \mu) = (\gamma, 0)$ is invalid. Hence we consider a more universal expression for κ_{eff} , which is based on entropy generation. When the total heat exchange is Q , the total entropy input from the heat baths is given by $Q(T^{-1}|_{x=0} - T^{-1}|_{x=L})$. According to the entropy balance, it should be offset by the total entropy production $\int \Phi dt$, namely,

$$Q \left(\frac{1}{T|_{x=0}} - \frac{1}{T|_{x=L}} \right) = - \int \Phi dt. \quad (3.2)$$

Thereupon, κ_{eff} is calculated as

$$\kappa_{eff} = -\frac{qL}{\Delta T} = -\frac{L}{A\Delta T} \frac{dQ}{dt} = \frac{\Phi L}{A} \frac{(T|_{x=0})(T|_{x=L})}{(\Delta T)^2}, \quad (3.3)$$

with A the cross-sectional area. The entropy production rate by the FFPE is given by

$$\Phi(\mu) = k_B K_{(1,\mu)} \int_0^L \left({}^L D_x^{\mu+1} P_\mu \right) \frac{\partial}{\partial x} (\ln P_\mu) dx, \quad (3.4)$$

where P_μ is the stationary or quasi-stationary solution for a given μ . When $\mu = 0$, κ_{eff} formulated by Eq. (3.3) should coincide with Fourier's law, and we have

$$\frac{\kappa_{eff}}{\kappa} = \frac{\Phi}{\Phi(\mu=0)} = \frac{K_{(1,\mu)}}{K_{(1,0)}} \frac{\int_0^L \left({}^L D_x^{\mu+1} P_\mu \right) \frac{\partial}{\partial x} (\ln P_\mu) dx}{\int_0^L \frac{\partial P_{\mu=0}}{\partial x} \frac{\partial}{\partial x} (\ln P_{\mu=0}) dx}. \quad (3.5)$$

Set $\xi = x/L$, and according to the Cauchy mean value theorem, there exists a $\xi_0 \in [0, 1]$ which fulfills

$$\frac{\kappa_{eff}}{\kappa} = \frac{\Phi}{\Phi(\mu=0)} = \frac{K_{(1,\mu)}}{K_{(1,0)} L^\mu} \left[\frac{\left({}^L D_\xi^{\mu+1} P_\mu \right) \frac{\partial}{\partial \xi} (\ln P_\mu)}{\frac{\partial P_{\mu=0}}{\partial \xi} \frac{\partial}{\partial \xi} (\ln P_{\mu=0})} \right] \Big|_{\xi=\xi_0}. \quad (3.6)$$

Eq. (3.6) means $\kappa_{eff} \sim L^{-\mu}$, and upon substituting $\beta = 2/(\mu+2)$, we obtain $\alpha = 2 - 2/\beta$. For arbitrary (γ, μ) , the above approach can also be adopted,

$$\frac{\kappa_{eff}}{\kappa} = \frac{\Phi_{(\gamma,\mu)}}{\Phi_{(1,0)}}, \quad \Phi_{(\gamma,\mu)} = k_B K_{(\gamma,\mu)} \int_0^L \left({}^{RL} D_t^{1-\gamma} {}^L D_x^{\mu+1} P \right) \frac{\partial}{\partial x} (\ln P) dx. \quad (3.7)$$

Through similar derivations, one can derive $\kappa_{eff} \propto t^{\gamma-1} L^{-\mu}$, and if the cut-off $t_C \propto L$ is used, it becomes $\kappa_{eff} \propto L^{\gamma-\mu-1}$. $(\gamma - \mu - 1)$ can be nonzero when $\beta = 2\gamma/(\mu+2) = 1$, which enables length-dependent κ_{eff} to coexist with the Brownian MSD $\langle |\Delta x|^2 \rangle \propto t$.

4. Summary

In summary, anomalous heat conduction in the presence of non-Brownian MSD is investigated by the FFPE with orders (γ, μ) , and κ_{eff} is derived as $\kappa_{eff} \propto t^{\gamma-1} L^{-\mu}$. Two classical relations between the anomaly $\kappa_{eff} = \kappa_{eff}(t, L)$ and long-time asymptotics $\langle |\Delta x|^2 \rangle \sim t^\beta$ are thus unified: $\kappa_{eff} \propto t^{\beta-1}$ corresponding to memory, while $\kappa_{eff} \propto L^{2-2/\beta}$ for nonlocality. In Ref. [8], $\kappa_{eff} \propto L^{2-2/\beta}$ arises from $\kappa_{eff} \propto L^2/t_{MFPT}$, where t_{MFPT} denotes the MFPT and obeys the scaling $t_{MFPT} \propto L^{2/\beta}$. If we select the MFPT as the cut-off time in the time-dependence $\kappa_{eff} \propto t^{\beta-1}$, the time-dependence becomes $\left(\kappa_{eff} \big|_{t=t_C} \right) \propto t_C^{\beta-1} \propto L^{2-2/\beta}$. It agrees with the spatial fractional-order case exactly. Hence, the two different scaling behaviors, $\kappa_{eff} \propto t^{\beta-1}$ and $\kappa_{eff} \propto L^{2-2/\beta}$, will lead to the same anomaly in the first passage theory. The FFPE predicts anomalous yet Brownian heat conduction that length-dependent κ_{eff} coexists with the Brownian MSD. Furthermore, the effective thermal conductivity formulated by the entropy production rate does not rely on local equilibrium or near equilibrium, which is necessary for the conventional linear response theory.

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