Brownian Motion Description of Heat Conduction by Phonons

K. Razi Naqvi and S. Waldenstrøm
Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway
(Received 7 April 2005; published 5 August 2005)

A non-Markovian partial differential equation, rooted in the theory of Brownian motion, is proposed for describing heat conduction by phonons. Although a finite speed of propagation is a built-in feature of the equation, it does not give rise to an inauthentic wave front that results from the application of Cattaneo's equation. Even a simplified, analytically tractable version of the equation yields results close to those found by solving, through more elaborate means, the equation of phonon radiative transfer.

DOI: 10.1103/PhysRevLett.95.065901 PACS numbers: 66.70.+f, 02.70.Uu, 05.40.−a, 05.60.Cd

Thermal conduction has been treated, until quite recently, within the framework of the classical parabolic heat equation, associated with the name of Fourier, or by using the hyperbolic heat equation, frequently named after Cattaneo [1]. The failure of Fourier's equation, which becomes apparent when one examines heat conduction on small scales [2–5], is easily grasped, for it implies an infinite speed of heat propagation; more disappointing, however, is the failure, under similar circumstances, of Cattaneo's equation, since it does assign a finite value to the speed of propagation. Recognition of the inadequacies of these equations prompted Majumdar [2] to introduce an equation that has come to be known as the equation of phonon radiative transfer (EPRT); it models conduction of heat in thin dielectric films as the transport of phonons, in analogy with the linear Boltzmann equation (LBE) used for describing the transport of photons and monoenergetic neutrons [6]. Since even simple versions of EPRT are time consuming [3], one is tempted to replace it with an easier alternative that is more trustworthy than the equations of Fourier and Cattaneo. Recently, Chen has proposed a promising approach, to be labeled here as the ballistic-diffusive approximation (BDA), where Cattaneo's equation is grafted onto the collisionless form of EPRT [4,5]. An unsatisfactory feature of BDA, traceable to Chen's employment of Cattaneo's equation, is the occurrence of an artificial wave front in the diffusive component of the internal energy. Another manifestation of the distortion introduced by Cattaneo's equation is a small but significant disagreement between the temperature profiles predicted by EPRT and BDA.

In this Letter, we propose a new heat equation (NHE) for describing phonon-mediated heat conduction, and present results obtained by employing an analytically tractable version of the equation. Since we wish to compare our results with those reported by other workers [3–5], we will treat a plane-parallel conducting medium. We will denote the average speed of sound by v and the mean-free path of phonons by ℓ; the symbol $\tau \equiv \ell/v$ will be called the mean-free time.

The general form of NHE will be presented after we have examined an exactly soluble special case that can be written as

$$\partial_t T(x, t) = (1 - e^{-t/\tau})\kappa \partial_{xx} T(x, t), \tag{1}$$

where $\partial_y \equiv \partial/\partial y$ and $\partial_{yy} \equiv \partial_y \partial_y$; $T(x, t)$ denotes the temperature at time t at the point x, and $\kappa = v\ell/3$ is thermal diffusivity. One sees immediately that Eq. (1) reduces to Fourier's equation, $\partial_t T = \kappa \partial_{xx} T$, in the long-time limit ($e^{-t/\tau} \ll 1$); furthermore, the substitution $s = t - \tau(1 - e^{-t/\tau})$ reduces Eq. (1) to $\partial_s T = \kappa \partial_{xx} T$.

To begin with the statement of the problem: A slab of thickness L is initially at a uniform temperature T_0; at time $t = 0$, one face (say, that at $x = 0$) is raised to a temperature T_1 and is maintained at this temperature thereafter, the other face (at $x = L$) being kept at the temperature T_0; we wish to find the temperature $T(x, t)$ and the flux $q(x, t)$, for $t > 0$ and $0 \le x \le L$. Since the problem has already been treated in the past [3–5], we will not give more details other than spelling out our notation: $\Delta T = T_1 - T_0$, $\xi = x/L$, $t^* = t/\tau$, $s^* = s/\tau$, $\theta = (T - T_0)/\Delta T$, $\phi = q/(Cv\Delta T)$, $\mathrm{Kn} = \ell/L$; Kn is the Knudsen number and C stands for the specific heat per unit volume.

It will be convenient to append to θ and ϕ an appropriate suffix (P, H, or N, depending on whether the result pertains to the parabolic, hyperbolic, or new heat equation). The equations used for calculating $\theta_P(\xi, t^*)$, $\theta_H(\xi, t^*)$, $\phi_P(\xi, t^*)$, and $\phi_H(\xi, t^*)$ have been stated (with some misprints) by previous authors [3,5]. The transformation $s = t - \tau(1 - e^{-t/\tau})$ enables us to express $\theta_N(\xi, t^*)$ and $\phi_N(\xi, t^*)$ as follows:

$$\theta_N(\xi, t^*) = \theta_P(\xi, s^*), \tag{2}$$

$$\phi_N(\xi, t^*) = (1 - e^{-t^*})\phi_P(\xi, s^*). \tag{3}$$

Figure 1 compares the performance of NHE with the other equations mentioned above; here the nondimensional temperature $\theta(\xi, t^*)$ and the nondimensional heat flux $\phi(\xi, t^*)$ are plotted against ξ at $t^* = 1$ in a slab for which $\mathrm{Kn} = 1$. It is to be noted that Chen [4,5] has rescaled his data so as to harmonize the definitions pertaining to the different equations; in the absence of such rescaling the EPRT plots show jumps at the boundaries (see below). One sees that the temperature profile predicted by NHE is in

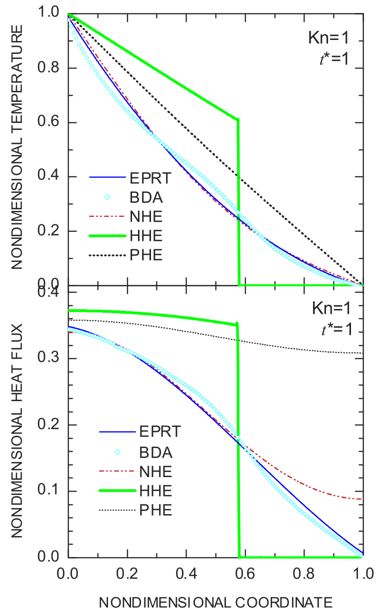

FIG. 1 (color online). Comparison of the spatial profiles of $\theta(\xi, t^*)$ and $\phi(\xi, t^*)$ calculated by using the equation of phonon radiative transfer (EPRT), Chen's ballistic diffusive approximation (BDA), the parabolic heat equation of Fourier (PHE), the hyperbolic heat equation of Cattaneo (HHE), and Eq. (1), the new heat equation (NHE). The data for the curves labeled EPRT and BDA have been taken from Refs. [4,5].

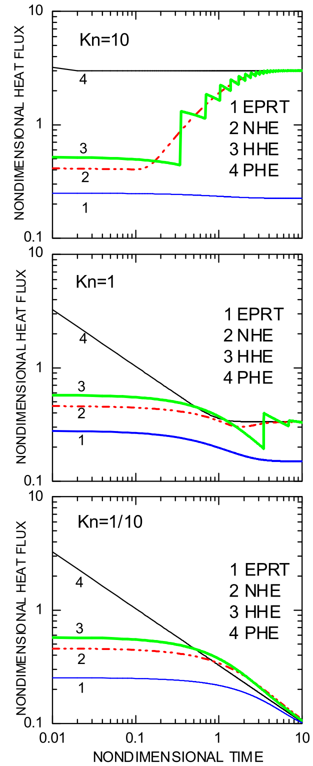

FIG. 2 (color online). Comparison of the temporal profile of the heat flux at $\xi = 0$ calculated by using EPRT, PHE, HHE, and NHE; the BDA data (not shown) are almost superposable on EPRT curves; for an explanation of the labels, refer to Fig. 1. The EPRT data have been read from Refs. [4,5].

excellent agreement with the rescaled EPRT plots; the flux predicted by NHE deviates visibly from the EPRT plot (for $\xi > 0.7$), but the other two plots (the parabolic heat equation of Fourier and the hyperbolic heat equation of Cattaneo) are in severe disagreement with the EPRT plot for nearly all values of ξ.

Curves showing the surface heat flux $\phi(0, t)$ are plotted in Fig. 2, and compared with reconstructions of Chen's plots. The top panel refers to a slab that is so thin that transport becomes essentially ballistic; this issue needs closer attention than can be paid here, but physical considerations lead us to expect that Eq. (4), given below, will perform better than Eq. (1). The middle and bottom panels of Fig. 2 reveal a persistent discrepancy between NHE and EPRT; this is to be expected since the EPRT data originate from plots which have not been rescaled.

Let us pause briefly to note that Eq. (1) provides, in all cases, a better description than that furnished by Cattaneo's equation. This means that the performance of BDA can be improved by discarding the Cattaneo equation in favor of Eq. (1). We return now to Eq. (1) and investigate the prospects of using it as a complete equation in itself; for this purpose, we will not consider samples where transport is dominated by ballistic behavior.

One would expect, in view of some previous investigations [2,3,7], temperature jumps to occur at the boundaries of sufficiently thin samples. To cope with temperature jumps, we must replace the boundary conditions $\theta(0, t^*) = 1$ and $\theta(1, t^*) = 0$ with $\theta(-\xi_0, t^*) = 1$ and $\theta(1 + \xi_1, t^*) = 0$, respectively. Postponing the issue of how the values of the *extrapolated end points* ($x_0 \equiv L\xi_0$ and $x_1 \equiv L\xi_1$) are to be found, we will estimate their values by using the results published by Chen [5]; it is pertinent to recall that, in the steady state, the diffusive part of his solution satisfies Marshak's boundary condition [6]: $x_0 = x_1 = 2\ell/3$, or equivalently $\xi_0 = \xi_1 = 2\mathrm{Kn}/3$.

Let us consider now a slab for which $\mathrm{Kn} = 0.1$ and focus attention on the temperature profiles at the instants $t^* = 1$, 10, and 100. An examination of Chen's EPRT plot for $t^* = 100$, which is almost linear, shows that ξ_0 and ξ_1 are, as one would expect from the above remark concerning the boundary conditions, close to 0.07 [5]. By choosing $\xi_0 = 0.07 = \xi_1$, we were led to plots that agreed well, for $t^* = 10$ and $t^* = 100$, with the EPRT counterparts in Chen's work; but for $t^* = 1$, a sufficiently close fit to the EPRT values could not be obtained without changing ξ_0 to 0.03. For substantiating these statements, we draw the reader's attention to the upper panel of Fig. 3, where our plots are compared with Chen's BDA curve ($t^* = 100$) or with his EPRT plots ($t^* = 1$ and 10). To avoid clutter, we have not displayed the BDA values for $\xi > 0.4$, and we have also chosen not to reproduce Chen's EPRT plot (for $t^* = 100$), which is close to the NHE plot for all values of ξ and to

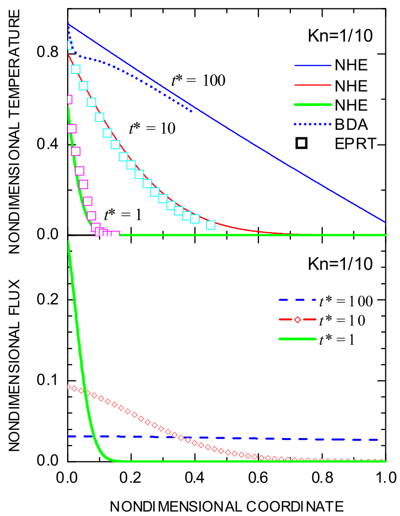

FIG. 3 (color online). Profiles of $\theta(\xi, t^*)$ (upper panel) and $\phi(\xi, t^*)$ (lower panel) as predicted by NHE. The open squares represent the prediction of EPRT (for $t^* = 1$ and 10) reported in Ref. [5]. The dotted curve, derived from a plot in Ref. [5], is the output (for $t^* = 100$) of BDA.

BDA for $\xi > 0.2$. We would like to add here that it did not seem worthwhile to improve the fit by fine-tuning the inputs for the extrapolated end points. Finally, we show, in the lower panel of Fig. 3, our plots for $\phi(\xi, t^*)$ for three particular instants ($t^* = 1$, 10, and 100), using the same values of ξ_0 as those mentioned above (0.03, 0.07, and 0.07, respectively). The plots for $t^* = 10$ and $t^* = 100$ are in notable agreement with Chen's EPRT plots; the shape of the flux plot at $t^* = 1$ accords with its EPRT counterpart, but its initial amplitude is larger. We believe that this is due, at least in part, to inappropriate choices for the extrapolated end points.

The foregoing evidence leads us to conclude that Eq. (1) affords an exceptionally simple, stand-alone strategy for studying transient heat conduction in a system where precise values of the extrapolated end points are not needed. On the basis of the results presented in Fig. 3 and some arguments given later, we suggest that this requirement will be met when Kn $\leq 1/10$ and $t^* \geq 10$.

Having illustrated the performance of an analytically tractable form of NHE, we now state its general form,

$$\partial_t T(x,t) = \frac{1}{2} a(t)\partial_{xx} T(x,t) - b(t)\partial_x T(x,t), \qquad (4)$$

and hasten to add that the equation is new only in the context of heat conduction; if $T(x,t)$ is replaced by $F(x,t)$, the probability density of a particle in coordinate space, Eq. (4) becomes identical with an equation of Ornstein and van Wijk [8]. The physical significance of $a(t)$ and $b(t)$ is easily grasped by considering an infinite space system and subjecting Eq. (4) to a Fourier transformation, which yields $\partial_t \hat{T}(k,t) = -\frac{1}{2}k^2 a(t)\hat{T}(k,t) - \iota k b(t)\hat{T}(k,t)$, where $\hat{T}(k,t) \equiv \int_{-\infty}^{\infty} dx \exp(-\iota k x) T(x,t)$. With $m(t) = \int_0^t b(t_1)dt_1$ and $\sigma^2(t) = \int_0^t a(t_1)dt_1$, one gets $\hat{T}(k,t) = \exp[-\{\iota k m(t) + \frac{1}{2}k^2\sigma^2(t)\}]\hat{T}(k,0)$; the fundamental solution to Eq. (4), corresponding to the initial condition $T(x,0) = \delta(x - x_i)$, is a Gaussian with a mean $m(t)$ and a variance $\sigma^2(t)$. Physically, m is the distance covered in time t with a mean velocity b, and σ is the corresponding dispersion; at long times, b vanishes and a attains a constant value; the time-dependence of a and b chronicles the ballistic phase of the motion. A phase-space description (involving both position x and velocity $\dot{x}$) of a Markovian process becomes, when projected on x space, non-Markovian, and initial data enter the reduced equation itself in the form of time-dependent coefficients [8,9]; at sufficiently long times, even the reduced description takes a Markovian appearance, which accounts for the success (and the limitation) of Fourier's equation. Since Eq. (4) holds only for a Gaussian process with white noise [8,9], it can merely approximate EPRT (see below).

A great merit of Majumdar's contribution [2] is that it provides a concrete basis for pursuing the analogy between phonon-mediated heat conduction and particle diffusion in terms of the relevant equations. In the original formulation of EPRT, the speed of phonons is taken to be a constant, but the mean-free time is viewed as an ω-dependent quantity, where ω ($0 \leq \omega \leq \omega_D$) denotes the frequency. However, in the simplified version used in Refs. [3–5] and under scrutiny here, the ω dependence of the mean-free time is ignored. With a constant mean-free time (denoted here by τ), EPRT can be converted, through integration over ω, into an equation for $g(x,\mu,t) \equiv \int_0^{\omega_D}[I_\omega(x,\mu,t)/v]d\omega$ that has the same form as LBE with isotropic scattering, which may be written as $[\partial_t + v\mu\partial_x]\psi(x,\mu,t) = \alpha(\frac{1}{2}\mathcal{P} - 1) \times \psi(x,\mu,t)$, where $\mathcal{P} \equiv \int_{-1}^{1} d\mu$. This implies that the internal energy $U(x,t) = \mathcal{P}g(x,\mu,t)$ and the heat flux $q(x,t) = v\mathcal{P}\mu g(x,\mu,t)$ are the analogs of $F(x,t) = \mathcal{P}\psi(x,\mu,t)$ and $J(x,t) \equiv v\mathcal{P}\mu\psi(x,\mu,t)$, respectively. To accommodate the concept of temperature, we recall Chen's definition [5], $T(x,t) = U(x,t)/C$, and stress that a different definition would invalidate the rest of the argument.

Let $\overline{x^n}^{\mu_i} \equiv \int_{-\infty}^{\infty} dx \int_{-1}^{1} d\mu x^n \psi(x,\mu,t; x_i,\mu_i)$, where x_i and μ_i denote the initial values of x and μ, respectively; we will assume, without sacrificing generality, that all particles start with the same value of x_i, since a subsequent integration over the distribution of x_i can always be performed, and the variance of x is independent of x_i. With $X \equiv x - \bar{x}^{\mu_i}$, we define the nth central moment of x as $\overline{X^n}^{\mu_i}$. One can use LBE to calculate the central moments [10], and it turns out that $\overline{X^3}^{\mu_i} \neq 0$ and $\overline{X^4}^{\mu_i} \neq 3[\overline{X^2}^{\mu_i}]^2$. Using the suffixes RT and BM to denote radiative transport and Brownian motion, respectively, the situation can be summed up as follows: X_{RT} does not have a Gaussian distribution but X_{BM} does. Thus, Eq. (4) cannot provide an exact description of radiative transfer. The simplified treatment advocated here is achieved by insisting that X_{RT} is Gaussian; once this concession is made, phonon radiative transfer can be treated as a boundary value problem within the framework of Eq. (4), with $m = \bar{X}^{\mu_i}$ and $\sigma^2 = \overline{X^2}^{\mu_i}$. A Gaussian approximation for photons was recently proposed [11], but it was not related to Eq. (4).

We return now to Eq. (4) and point out that the expressions for $a(t)$ and $b(t)$ depend on how phonons are injected at the surface $x = 0$ [10]. If $\mu_i = 1$ (initial velocity parallel to the x axis), one gets $b(t) = ve^{-t^*}$ and $a(t) = \kappa[2 - 8E + 4Et^* + 6E^2)]$, with $E \equiv e^{-t^*}$. A second special case, which leads to Eq. (1), is that of an isotropic distribution of μ_i; for this situation, $b(t) = 0$ and $a(t) = 2\kappa(1 - e^{-t^*})$. We chose to work with Eq. (1) mainly because of the resulting reduction in labor, but in part because we wish to present it as a substitute for Cattaneo's equation, which is discussed below.

When integrated over all μ, LBE leads to the continuity equation, $\partial_t F + \partial_x J = 0$; when multiplied by $v\mu$ and integrated over all μ, LBE gives $\tau\partial_t J + J = -v^2\tau\partial_x \mathcal{P}\mu^2\psi(x, \mu, t)$. If one assumes that $\mathcal{P}\mu^2\psi(x, \mu, t) = \frac{1}{3}F(x, t)$, the second relation becomes $\tau\partial_t J + J = -(v^2\tau/3)\partial_x F$ and yields, if combined with the first, $[\tau\partial_{tt} + \partial_t]F = (v^2\tau/3)\partial_{xx}F$, a relation named the telegrapher equation or Cattaneo's equation (depending on the context). Cattaneo's equation and Eq. (1) are approximations to EPRT, but Eq. (1) is far superior, as shown above, because it has no second-order time derivative. Even if the phonons are incident normally at the surface $x = 0$, their velocity distribution will randomize after a few mean-free times, and Eq. (1) will begin to furnish an adequate account of phonon transport, hence the aforementioned restrictions concerning its use.

We will now make a brief allusion to the Milne problem, which is exactly soluble for three linear transport equations [12]: the Klein-Kramers equation, the single-relaxation time approximation to the Boltzmann equation, and LBE. The problem itself may be stated as follows [12]: A homogeneous, semi-infinite, nonabsorbing medium occupies the half-space $x > 0$, and sustains a constant current of particles in the negative x direction, the region $x < 0$ is vacuum, and no particles hit the surface $x = 0$ in the positive x direction; the problem is to determine the particle density in the region $x > 0$. Though each equation describes a different physical system, the respective plots of $F(x, t)$ against x have the same overall appearance; indeed, within the lowest-order diffusion approximation, all three imply a rectilinear plot with the same extrapolated end point; higher-order approximations, or the exact solutions, do reveal residual differences. Given this background, one expects the temperature profile predicted by Eq. (4) to be close, but not identical, to that found by using EPRT. We would like to mention here the possibility, to be explored in the future, of introducing some corrections to Eq. (4) by using the higher central moments [10] or by making *ad hoc* changes in the expressions for $a(t)$ and $b(t)$.

All that remains is to discuss the boundary conditions to be imposed on the solutions of Eqs. (1) and (4). Since there is some disagreement about this matter in the field of heat conduction [5], we will content ourselves by drawing attention to a few relevant contributions concerning Milne's problem [13–15]; particularly relevant in this context is the finding that the extrapolated end point is a time-dependent quantity.

[1] D. D. Joseph and L. Preziosi, Rev. Mod. Phys. **62**, 375 (1990).
[2] A. Majumdar, J. Heat Transfer **115**, 7 (1993).
[3] A. A. Joshi and A. Majumdar, J. Appl. Phys. **74**, 31 (1993).
[4] G. Chen, Phys. Rev. Lett. **86**, 2297 (2001).
[5] G. Chen, J. Heat Transfer **124**, 320 (2002).
[6] J. J. Duderstadt and W. R. Martin, *Transport Theory* (Wiley, New York, 1979).
[7] T. Klitsner, J. E. VanCleve, H. E. Fischer, and R. O. Pohl, Phys. Rev. B **38**, 7576 (1988).
[8] L. S. Ornstein and R. van Wijk, Physica (Utrecht) **1**, 235 (1933).
[9] M. San Miguel and J. M. Sancho, J. Stat. Phys. **22**, 605 (1980).
[10] K. Razi Naqvi, cond-mat/0504429.
[11] M. Xu, W. Cai, M. Lax, and R. R. Alfano, Phys. Rev. E **65**, 066609 (2002).
[12] For a review, see K. Razi Naqvi, in *Condensed Matter Theories*, edited by J. W. Clark, K. A. Shoaib, and A. Sadiq (Nova, Commack, NY, 1994), Vol. 9, p. 218.
[13] K. Razi Naqvi, K. J. Mork, and S. Waldenstrøm, Phys. Rev. Lett. **49**, 304 (1982).
[14] S. V. G. Menon and D. C. Sahni, Phys. Rev. A **32**, R3832 (1985).
[15] S. V. G. Menon, V. Kumar, and D. C. Sahni, Physica (Amsterdam) **135A**, 63 (1986).