Memory and nonlocal effects of heat transport in a spherical nanoparticle

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Abstract. In this paper a mathematical model describing the heat transport in a spherical nanoparticle subject to Newton heating at its surface is presented. The governing equations involve a phonon hydrodynamic equation for the heat flux and the classical energy equation that relates the heat flux and the temperature. Assuming radial symmetry the model is reduced to two partial differential equation, one for the radial component of the flux and one for the temperature. We solve the model numerically by means of finite differences. The resulting temperature profiles show characteristic wave-like behaviour consistent with the non Fourier components in the hydrodynamic equation.

1. Introduction

It is well known that Fourier law breaks down at length scales of the order of the phonon mean free path and time scales of the order of the relaxation time of the heat carriers. Recently, solutions of the classical heat transfer model describing melting and solidification were compared with molecular dynamics simulations [1, 2], observing deviations at times below 100 ps and length scales ranging from 20 to 40 nm. The breakdown of the Fourier law has important ramifications due to the current trend of miniaturization of electronic devices [3]. Understanding the fundamentals of heat flow at the nanoscale is necessary to improve thermal management of micro/nano electronic devices and for the design of new materials for energy conversion.

The phonon hydrodynamic model, derived from the Boltzmann transport equation [4, 6, 7, 8, 9, 10], is an effective macroscopic heat equation that accounts for non Fourier deviations occurring at extremely small scales and ultrafast heating conditions. The phonon hydrodynamics equation for the heat flux $\mathbf{q}$ is

$$\tau_R \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -k\nabla T + \frac{1}{5}\Lambda^2\left[\nabla^2\mathbf{q} + \frac{1}{3}\nabla(\nabla\cdot\mathbf{q})\right] \tag{1}$$

where τ_R is the phonon relaxation time, k the thermal conductivity, Λ the phonon mean free path, ρ the density and c the specific heat [5]. The connection between the heat flux and the temperature T is established by means of the energy equation

$$\rho\, c\,\frac{\partial T}{\partial t} + \nabla\cdot\mathbf{q} = 0\,. \tag{2}$$

2. Radially symmetric problem and solution method

In the current paper we are concerned with the heat transport in a spherical nanoparticle. Thus, we assume radial symmetry and write the equations for the radial component of the heat flux as

$$\tau_R \frac{\partial q}{\partial t} + q = -k\frac{\partial T}{\partial r} + \frac{4}{15}\,\Lambda^2 \frac{\partial}{\partial r}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 q\right)\right] \tag{3}$$

and the equation for the temperature as

$$\rho\, c\,\frac{\partial T}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 q\right) = 0\,. \tag{4}$$

We assume radial symmetry at $r = 0$ and a Newton heating boundary conditions at $r = R$, so

$$q(0,t) = 0\,, \qquad q(R,t) = h(T(R,t) - T_H)\,, \tag{5}$$

where h is a heat transfer coefficient. The initial conditions are

$$q(r,0) = 0\,, \qquad T(r,0) = T_0\,. \tag{6}$$

Operating (3) with ∇^2 and using equation (4), equations (3)-(4) can be written in a single equation for the temperature as follows

$$\tau_R \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \frac{k}{\rho\, c}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) + \frac{4}{15}\,\Lambda^2\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial^2 T}{\partial r\partial t}\right)\,. \tag{7}$$

Although we will not use (7) when solving the model, it is illustrative to understand the wave-like phenomena observed in the results section.

2.1. Nondimensional form and numerical solution

We take the dimensionless variables

$$\hat{T} = \frac{T - T_0}{\Delta T}\,, \qquad \hat{q} = \frac{q}{Q}\,, \qquad \hat{r} = \frac{r}{R}\,, \qquad \hat{t} = \frac{t}{\tau} \tag{8}$$

where $\Delta T = T_H - T_0$, $Q = h\Delta T$ and $\tau = \rho c R \Delta T/Q$. Dropping the hat notation, the equations now read

$$\gamma\frac{\partial q}{\partial t} + q = -\lambda\frac{\partial T}{\partial r} + \frac{4}{15}\,\mathrm{Kn}^2\frac{\partial}{\partial r}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 q\right)\right] \tag{9}$$

$$\frac{\partial T}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 q\right) = 0 \tag{10}$$

with the boundary and initial conditions

$$q(0,t) = 0\,, \qquad q(1,t) = T(1,t) - 1\,, \qquad q(r,0) = 0\,, \qquad T(r,0) = 0\,. \tag{11}$$

The nondimensional parameters are

$$\gamma = \frac{\tau_R}{\tau}\,, \qquad \lambda = \frac{k}{hR}\,, \qquad \mathrm{Kn} = \frac{\Lambda}{R}\,. \tag{12}$$

The problem (9)-(11) is solved numerically using a forward in time and central in space finite difference scheme that we implement in Matlab.

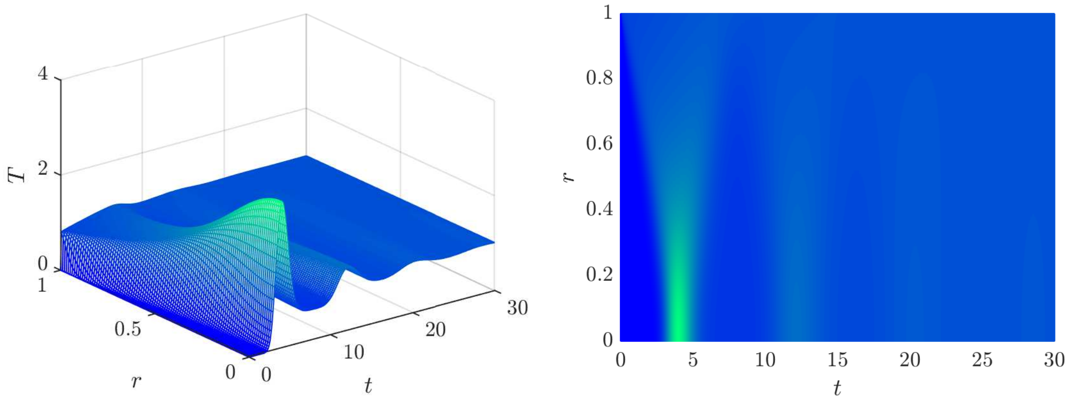

Figure 1. Temperature maps in space and time for $\gamma = 8$, $\mathrm{Kn} = 0.5$, $\lambda = 0.5$.

3. Results

In Figure 1 we show space-time maps of the temperature for the set of parameters $\gamma = 8$, $\mathrm{Kn} = 0.5$ and $\lambda = 0.5$. The left panel shows a wave-like temperature evolution consistent with a second time derivative in (7). The panel on the right shows a clear periodic patter, with temperature peaks occurring at around $t \approx 4$, $t \approx 13$ and $t \approx 20$.

In Figure 2 we present the evolution of the temperature at the centre and at the surface of the nanoparticle (left panel) and temperature profiles along the radius at different times (right panel). In the left panel we observe a large temperature peak at very early times, which periodically appears increasingly attenuated at times $t \approx n\, t_c$, where $t_c \approx 4$ is a characteristic time and n a positive integer number. The temperature profiles in the right panel show a wave front that travels inwards towards the center of the particle first and outwards towards the nanoparticle surface after.

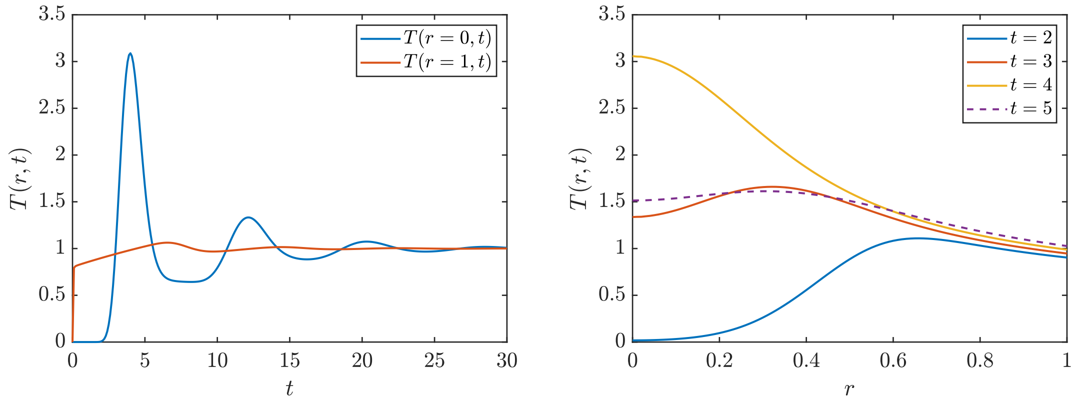

Figure 2. Temperature evolution at $r = 0$ and $r = 1$ (left panel) and temperature profiles at several times (right panel) for the parameter set $\gamma = 8$, $\mathrm{Kn} = 0.5$, $\lambda = 0.5$.

4. Conclusions

In this work, we have formulated the spherically symmetric version of the phonon hydrodynamic equation to model the temperature evolution in a nanoparticle. The equation is solved numerically by means of finite differences for a specific set of parameters that illustrate a situation where the phonon mean free path and the heat relaxation time are the representative length and time scales of the system, respectively. In this situation, the memory and nonlocal effects play a dominant role in the heat propagation, and the temperature reveals a strong wave-like behaviour.

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