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Time-fractional heat equations and negative absolute temperatures

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ABSTRACT

The classical parabolic heat equation based on Fourier's law implies infinite heat propagation speed. To remedy this physical flaw, the hyperbolic heat equation is used, but it may instead predict temperatures less than absolute zero. In recent years, fractional heat equations have been proposed as generalizations of heat equations of integer order. By simulating a 1D model problem of size on the order of a thermal energy carrier's mean free path length, we have done a study of four fractional generalized Cattaneo equations from Compte and Metzler (1997) called GCE, GCE I, GCE II, and GCE III and also a fractional version of the parabolic heat equation. We have observed that when the fractional order is large enough, these equations give temperatures less than absolute zero. But if the fractional order is small enough, GCE I does not have this problem when the domain length is comparable to the mean free path length. With larger size, GCE I and GCE III also give non-oscillating solutions for both small and large values of the fractional order.

1. Introduction

The classical parabolic heat equation (PHE) based on Fourier's law is widely used in engineering. This equation implies that the heat propagation is of infinite speed [1,2]. To obtain finite thermal propagation speed, Cattaneo's equation [3] has been used in place of Fourier's law. It gives a hyperbolic heat equation (HHE). However, researchers have shown that the HHE, although it solves one problem, may introduce other non-physical properties. Bai and Lavine [4] noticed that it could give temperatures less than absolute zero if the size of the domain is on the order of a phonon's mean free path. Körner and Bergmann [5] demonstrated that the reason that it gave an unphysical solution was that the hyperbolic approach to heat current density violated the fundamental law of energy conservation. Rubin [6] also proved that Cattaneo's equation may violate the second law of thermodynamics since it may predict heat flowing from cold to hot regions in a finite time period. It should also be noted that there are alternative approaches to incorporate a finite propagation speed, such as random walks [7], the molecular dynamics model [8], the phonon radiative transfer model [9], and so on.

In recent years, several researchers have introduced fractional heat flux models which lead to fractional heat equations. Compte and Metzler [1] proposed time fractional generalized Cattaneo equations (GCEs), and each one was supported by continuous time random walks, non-local transport theory, and delayed flux-force relation. Povstenko [10] followed Compte and Metzler's work and formulated the corresponding theory of thermal stresses. Metzler and Klafter [11] also gave a general physical introduction to fractional equations. Just recently, Qi et al. [12] used the fractional Cattaneo model to simulate laser short-pulse heating of a solid surface.

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Following Bai and Lavine [4], an interesting question is whether fractional heat equations also can give temperatures less than absolute zero. In this paper, we use numerical solutions to show that like the hyperbolic heat equation, fractional heat equations may also give temperatures less than absolute zero under certain conditions.

2. Background

The purpose of this section is to summarize the equations that will be studied numerically later. These equations are obtained from earlier published papers.

2.1. Parabolic and hyperbolic heat equations

The classical parabolic heat equation is based on the Fourier heat conduction equation:

$$\mathbf{q} = -k\nabla T. \tag{1}$$

Eq. (1) is a unifying form of Fourier's law, Fick's law and Darcy's law but only with different physical parameters. For example, in the diffusion theory, $\mathbf{q}$ is the matter flux vector, k is the diffusion conductivity, T is the concentration gradient. For Darcy's law, k is the conductivity of the porous material, T is the pressure in the fluid, $\mathbf{q}$ is the production of average velocity and the volume fraction of the fluid [13].

Combining (1) with the law of conservation of energy:

$$\rho_m c_m \frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{q}, \tag{2}$$

one gets the parabolic heat equation:

$$\frac{1}{a}\frac{\partial T}{\partial t} = \Delta T \quad \text{(PHE)}, \tag{3}$$

where $\mathbf{q}$ is the heat flux vector, T is the temperature, and k, ρ_m, c_m, $a = k/\rho_m c_m$ are thermal conductivity, density, specific heat capacity, and the thermal diffusivity respectively. We only consider isotropic and homogeneous thermal conductivity so the parameters do not depend on position or orientation. To obtain finite thermal propagation speed, Cattaneo proposed to add a relaxation term [3]:

$$\mathbf{q} + \tau\frac{\partial \mathbf{q}}{\partial t} = -k\nabla T. \tag{4}$$

Combining Cattaneo's equation (4) with (2), one obtains the hyperbolic heat equation:

$$\frac{1}{c^2}\frac{\partial^2 T}{\partial t^2} + \frac{1}{a}\frac{\partial T}{\partial t} = \Delta T \quad \text{(HHE)}, \tag{5}$$

where τ is the relaxation time and $c = \sqrt{a/\tau}$ is the thermal propagation speed. The hyperbolic heat equation can be said to be a damped wave equation.

Bai and Lavine [4] have pointed out that the hyperbolic heat equation gives unphysical results when the size of the domain is on the order of a thermal energy carrier's mean free path or less. The value for the mean free path is $l_{mfp} = 3a/c$. Likewise Rubin [6] gave the critical length as $L_{cr} = 2\pi a/c \approx 2l_{mfp}$ and estimated it to be about 10^{-6} m for silver.

2.2. Fractional heat equations

In recent decades, the classical theories such as Fourier's law, Fick's law and Darcy's law have been generalized. Gurtin and Pipkin [14] proposed that the law of heat conduction can be given by a general non-local dependence in time:

$$\mathbf{q}(t) = -k\int_0^\infty K(u)\nabla T(t-u)du. \tag{6}$$

Substituting $\tau = t - u$ and choosing 0 as a starting point of the integral, one gets a heat conduction equation with memory [10]:

$$\frac{\partial T}{\partial t} = a\int_0^t K(t-\tau)\Delta T(\tau)d\tau. \tag{7}$$

Fourier's law, Eq. (1) and the classical equation, Eq. (3), can be obtained by choosing the kernel function $K(t)$ as the Dirac delta function [10]. With a memory power law kernel, the flux can be interpreted in terms of fractional integrals and derivatives. This leads to the time fractional heat equation (FHE):

$$\frac{\partial^\gamma T}{\partial t^\gamma} = a\Delta T \quad (0 < \gamma \le 2) \text{ (FHE)}. \tag{8}$$