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FRACTIONAL HEAT EQUATION AND THE SECOND LAW OF THERMODYNAMICS

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Abstract

In the framework of second law of thermodynamics, we analyze a set of fractional generalized heat equations. The second law ensures that the heat flows from hot to cold regions, and this condition is analyzed in the context of the Fractional Calculus.

Mathematics Subject Classification: 35Q80, 35R11, 26A33

Key Words and Phrases: Second law of thermodynamics, Fractional heat equation, Fractional derivatives and integrals

1. Introduction

The general one dimensional space-fractional diffusion equation

$$\frac{\partial T}{\partial t} = k\frac{\partial^\beta T}{\partial x^\beta}, \qquad 1 < \beta \leq 2 \tag{1.1}$$

can be interpreted as a generalization of the heat equation ($\beta = 2$)

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} \tag{1.2}$$

The fractional derivative operators are non-local and this property is very important in the applications because it allows to model the dynamic of many complex processes in the applied sciences and engineering. The space-fractional diffusion equation (1.1) has been considered in the literature by numerous authors, see for instance [1], [2], [4], [5], [6], [8], [9], [13]. Also, the equation (1.1) represents a hyperbolic wave equation for $\beta = 1$ and a parabolic diffusion equation for $\beta = 2$, such that the equation (1.1) can

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be interpreted as the interpolation between a hyperbolic and a parabolic equation.

First of all, let us remember the well known deterministic approach to the one-dimensional heat equation. Therefore the heat Fourier model is based in three ideas for an one-dimensional system as a isolated bar:

- The energy that is necessary to change the temperature of a section ΔT of a bar from zero to T is proportional to $\Delta l T$. The energy density is proportional to the temperature
$$\epsilon = KT \tag{1.3}$$
with K a characteristic constant of the material.
- The energy flows from high temperature to low temperature regions, according to the second law of thermodynamics. Also the time rate of heat transfer through a material is proportional to the negative gradient in the temperature and to the area through which the heat is flowing
$$\phi = -\mu D_x T \tag{1.4}$$
where ϕ is the energy flux density, μ is a constant that is characteristic of the material and the minus sign ensures that the heat flows from hot to cold regions. This law is experimental and its name is Fourier Law in the case of the heat equation (the simplest case).
- The energy conservation law. In a section of the bar, Δl, the energy in Δl in the instant t_2 is equal to the energy in Δl in the instant t_1 plus the flux of energy that get in by the extremes x_1, x_2 of the Δl in the interval of time (t_1, t_2):
$$\int_{\Delta l} (\epsilon(x, t_2) - \epsilon(x, t_1))dx = \int_{t_1}^{t_2} (-\phi(x_2, t) + \phi(x_1, t))dt \tag{1.5}$$

Then, according to the conservation law, we have in general the constitutive equation
$$D_t \epsilon + D_x \phi = 0 \tag{1.6}$$
where as we indicated before $\epsilon = KT$ and $\phi = -\mu D_x T$ in the classical case. By using the relations (1.3) and (1.4) we get
$$D_t T = \frac{\mu}{K} D_{xx} T \tag{1.7}$$

How the heat flows in the medium is the key point to understand the fractional heat equation (1.1) with $1 < \beta = 1 + \rho \leq 2$. The classical diffusion equation is used for ordinary cases where a normal medium is considered and then a simple derivative allows to model ordinary phenomena. However in many cases, the processes take place in anomalous media (organic tissues, heterogeneous materials...) with characteristics that can affect the evolution of the energy flux [2], [6]. For example the heterogeneity of the medium is a factor that can modify the velocity of the flux, from a macroscopic and microscopic point of view, but it is natural that the second law of thermodynamics can not be modified. For this reason it is necessary to introduce a variation that allows us to characterize this type of complex processes. A possible way to model this variation is by the introduction of a fractional derivative in the energy flux density, such that this fractional derivative characterizes the strong abnormality of the medium through a kernel of convolution ([2], [12], [10]). For this objective we can use a deterministic approach and we can rewrite (1.4) in a integral form that represents a simple convolution [3]:

$$T(x,t) = \int_x^\infty \frac{\phi(\xi,t)}{\mu} d\xi + T(\infty,t) = 1 * \left(\frac{\phi(x,t)}{\mu}\right) \tag{1.8}$$

(we assume $T(\infty,t) = 0$). Then this expression can be generalized for different types of materials by introduction of a suitable kernel $K(x)$ instead of 1

$$T(x,t) = K(x) * \left(\frac{\phi(x,t)}{\mu}\right) \tag{1.9}$$

Depending on the considered medium, we could consider a kernel $K(x)$ associated to a fractional integral I_x^ρ (for example, we propose the kernel $K(x) = \frac{x^{\rho-1}}{\Gamma(\alpha)}$ that is related to the Liouville fractional integral, because this kernel characterizes many complex processes [2], [6], [10], [13]), where ρ is a parameter that will depend of the thermal properties of the material, and then we have

$$T(x,t) = K(x) * \left(\frac{\phi(x,t)}{\mu}\right) = I_x^\rho \left(\frac{\phi(x,t)}{\mu}\right) \tag{1.10}$$

that is equivalent to

$$\phi = -\mu D_x^\rho T. \tag{1.11}$$

Consequently the propagation of the temperature is governed by the equation

$$D_t T = \frac{\mu}{K} D_x^{1+\rho} T, \qquad 0 < \rho \leq 1 \tag{1.12}$$

(If $\rho = 0$, here we have a hiperbolic equation.)

Also, since the heat flux $\phi = -\mu \frac{\partial T}{\partial x}$ in the classical case verifies the second law of thermodynamics, the heat flux $\phi = -\mu D_x^\rho T$ of the new family of equations (1.12) will be compatible with the second law of thermodynamics if the following condition is satisfied ([11], [7])

$$D_x^\rho T \cdot \frac{\partial T}{\partial x} > 0 \tag{1.13}$$

Thus this property will restrict the possible fractional operators that can be considered in the generalized Fourier law and the initial and boundary conditions of the considered problem.

When $\rho = 1$ the condition (1.13) is trivial. But for $0 < \rho < 1$ it will be analyzed in the next section for two examples.

2. Fractional heat equation

As it is not easy to prove the condition (1.13) in general, we will study specific cases of the fractional heat equation, that is, we will use a specific fractional derivative and particular initial conditions. Let be the equation

$$\partial_t T = k\partial_x^{1+\rho} T, \qquad 0 < \rho \leq 1 \tag{2.1}$$

The solutions of the Cauchy problem associated to this equation are discussed by several authors, with different fractional derivative operators [2], [4].

2.1. With Liouville space-fractional derivative

Considering in this case $x \in \mathbb{R}$, we take the Liouville derivative operator that has the following expression, see for instance [12], [2]:

$$({}^L D^{\alpha}_{x,\infty} f)(x) = \frac{1}{\Gamma(n-\alpha)} \left(-\frac{d}{dx}\right)^n \int_x^{\infty} \frac{f(\xi)d\xi}{(\xi - x)^{\alpha-n+1}}, \qquad (x \in \mathbb{R}) \tag{2.2}$$

for $\alpha \in \mathbb{C}$, $\Re(\alpha) > 0$ and $n = [\Re(\alpha)] + 1$ $(n \in \mathbb{N})$, where $[\Re(\alpha)]$ means the integral part of $\Re(\alpha)$.

In this paper, we consider $0 < \rho \leq 1$ and then

$$({}^L D^{1+\rho}_{x,\infty} f)(x) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_x^{\infty} \frac{f(\xi)d\xi}{(\xi - x)^{\rho}}, \qquad (x \in \mathbb{R}) \tag{2.3}$$

So the generalized Cauchy problem in one dimension is:

$$D_t T(x,t) = k({}^L D^{1+\rho}_{x,\infty} T)(x,t), \quad 0 < \rho \leq 1, t > 0, x \in \mathbb{R}, k \in \mathbb{R}^+ \tag{2.4}$$

$$T(x, 0+) = g(x), \qquad x \in \mathbb{R} \tag{2.5}$$

$$\lim_{x \to \pm\infty} T(x,t) = 0, \qquad t > 0 \tag{2.6}$$

This problem is solvable and its solution is obtained applying the Laplace transform $\mathcal{L}_t$ with respect to $t > 0$

$$(\mathcal{L}_t u)(x,s) = \int_0^{\infty} u(x,t)e^{-st}dt, \qquad x \in \mathbb{R}, \quad s > 0 \tag{2.7}$$

and the Fourier transform $\mathcal{F}_x$ with respect to $x \in \mathbb{R}$

$$(\mathcal{F}_x u)(\sigma, t) = \int_{-\infty}^{\infty} u(x,t) e^{ix\sigma} dx, \qquad \sigma \in \mathbb{R}, \quad t > 0 \tag{2.8}$$

and using the following known formula for the Fourier transform of the fractional derivative [2]:

$$(\mathcal{F}_x(D^{\beta}_{x,\infty} T))(\sigma, t) = (i\sigma)^{\beta} (F_x T)(\sigma, t) \qquad (\beta > 0) \tag{2.9}$$

where

$$(i\sigma)^{\beta} := |\sigma|^{\beta} e^{\frac{\beta\pi i}{2} sign(\sigma)} \qquad (\sigma \in \mathbb{R}, \beta > 0) \tag{2.10}$$

This is a multi-valued function but the principal value will be taken.

So we obtain

$$(\mathcal{F}_x \mathcal{L}_t T)(\sigma, s) = \frac{\mathcal{F}_x g(\sigma)}{s - k(i\sigma)^{1+\rho}} \tag{2.11}$$

and applying the inverse Laplace and Fourier transform

$$(\mathcal{L}_t^{-1} u)(x,t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} u(x,s) ds, \qquad x \in \mathbb{R}, \quad s > 0 \tag{2.12}$$

$$(\gamma = \Re(s) > \text{abscisa de convergencia})$$

$$(\mathcal{F}_x^{-1} u)(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\sigma x} u(\sigma, t) d\sigma, \qquad \sigma \in \mathbb{R}, \quad t > 0 \tag{2.13}$$

the solution of this problem is (see [2] pp. 385)

$$T(x,t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} ds \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{(\mathcal{F}_x g)(\sigma)}{s - k(i\sigma)^{1+\rho}} e^{-i\sigma x} d\sigma \qquad (\gamma \in \mathbb{R}) \tag{2.14}$$

That is equivalent to

$$T(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{k(i\sigma)^{1+\rho} t} (\mathcal{F}_x g)(\sigma) e^{-i\sigma x} d\sigma \tag{2.15}$$

provided that the integrals in the right-hand sides of (2.14) and (2.15) exist.

Also in the case that g is a function in the space

$$\bar{S} = \{\varphi \in C^{\infty}(\mathbb{R}) : \lim_{|x| \to \infty} \varphi^{(m)}(x) = 0, m = 0, 1, 2...\} \tag{2.16}$$

then we can represent the exponential function as a power series, such that the uniform convergence allows to introduce the integral in the series, and finally the solution has the following form:

$$T(x,t) = \sum_{j=0}^{\infty} \frac{kt^j}{j!} ({}^{L}D^{(1+\rho)j}_{x,\infty} g)(x) \tag{2.17}$$

with the condition that this series converges for all $x \in \mathbb{R}$ and $t > 0$, and considering that this type of functions $g \in \bar{S}$ are continuous and the continuous functions verifies the indices law of the Liouville derivative.

Let us check if this solution verifies the condition (1.13). We need to compute the derivatives of the solution and these derivatives can be introduced into the series of the solution (2.17) because we have supposed this series converges:

$$({}^L D^{\rho}_{x,\infty} T)(x,t) = \sum_{j=0}^{\infty} \frac{kt^j}{j!} ({}^L D^{(1+\rho)j+\rho}_{x,\infty} g)(x) \tag{2.18}$$

$$\frac{\partial T}{\partial x}(x,t) = \sum_{j=0}^{\infty} \frac{kt^j}{j!} ({}^L D^{(1+\rho)j+1}_{x,\infty} g)(x) \tag{2.19}$$

2.1.1. *Particular solution for negative exponential initial condition:* Attending to this last expression, it is not possible to obtain restrictions of ρ in order to verify the condition (1.13) for all initial condition g. For this reason we will study the following particular case:

$$T(x,0+) = e^{-\lambda x}, \qquad \lambda > 0, x \in \mathbb{R} \tag{2.20}$$

Although this function does not belong to the space $\bar{S}$, it has the following property:

$$ {}^L D^{\alpha}_{x,\infty} e^{-\lambda x} = \lambda^{\alpha} e^{-\lambda x} \tag{2.21}$$

and then we can obtain the solution to the problem (2.4-2.5-2.6) easily as:

$$T(x,t) = e^{k\lambda^{1+\rho}t-\lambda x} \tag{2.22}$$

Consequently we have

$$({}^L D^{\rho}_{x,\infty} T)(x,t) = \lambda^{\rho} e^{k\lambda^{1+\rho}t-\lambda x} \tag{2.23}$$

$$\frac{\partial T}{\partial x}(x,t) = -\lambda e^{k\lambda^{1+\rho}t-\lambda x} \tag{2.24}$$

$$({}^L D^{\rho}_{x,\infty} T)(x,t) \cdot \frac{\partial T}{\partial x}(x,t) = -\lambda^{1+\rho} e^{2(k\lambda^{1+\rho}t-\lambda x)} < 0 \tag{2.25}$$

It is clear that in this case the condition (1.13) is not verified for all value of ρ.

2.1.2. *Particular solution for potential initial condition:* If we take the initial condition

$$T(x,0+) = x^{\gamma-1}, \qquad 0 < \gamma < 1, x \in \mathbb{R} \tag{2.26}$$

choosing γ such that the following property is verified:

$$ {}^{L}D^{\alpha}_{x,\infty} x^{\gamma-1} = \frac{\Gamma(1+\alpha-\gamma)}{\Gamma(1-\gamma)} x^{\gamma-\alpha-1}, \qquad \Re(\alpha - [\Re(\alpha)] + \gamma) < 1 \tag{2.27} $$

for all value $\alpha = (1+\rho)j$, $\alpha = (1+\rho)j+\rho$ and $\alpha = (1+\rho)j+1$, $j = 0, 1, 2, 3, ...$

As this function belongs to the space $\bar{S}$, the solution (2.17) has the form

$$ T(x,t) = \sum_{j=0}^{\infty} \frac{kt^j}{j!} \frac{\Gamma(1+(1+\rho)j-\gamma)}{\Gamma(1-\gamma)} x^{\gamma-(1+\rho)j-1} \tag{2.28} $$

Then

$$ ({}^{L}D^{\rho}_{x,\infty}T)(x,t) = \sum_{j=0}^{\infty} \frac{kt^j}{j!} \frac{\Gamma(1+(1+\rho)j+\rho-\gamma)}{\Gamma(1-\gamma)} x^{\gamma-(1+\rho)j-\rho-1} \tag{2.29} $$

$$ \frac{\partial T}{\partial x}(x,t) = \sum_{j=0}^{\infty} \frac{kt^j}{j!} \frac{\Gamma(2+(1+\rho)j-\gamma)}{\Gamma(1-\gamma)} x^{\gamma-(1+\rho)j-2} \tag{2.30} $$

Now, the condition (1.13) is reduced to

$$ ({}^{L}D^{\rho}_{x,\infty}T)(x,t) \cdot \frac{\partial T}{\partial x}(x,t) = \sum_{j=1}^{\infty} c_j \left(\frac{kt^j}{j!}\right)^2 x^{2\gamma-2-j(\rho+1)} \tag{2.31} $$

which is always positive for $\rho = 1$, but it is not possible to assure its positivity for $0 < \rho < 1$ in $x \in \mathbb{R}$ because negative values of x with real potentials appear in the result.

3. Conclusions

In this paper we give a motivation to introduce a space fractional derivative with parameter β in the heat equation. Such fractional generalization allows to model the anomalous properties of the medium, getting a generalization of the Fourier law. Then we study the second law of thermodynamics in this new fractional model and we introduce two examples where we can see that the use of the mentioned characterization is not trivial: we can find particular cases that do not verify the second law of thermodynamics and cases where it is not possible to assure that whether this law is verified.

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