

Fractional evolution Dirac-like equations: some properties and a discrete Von Neumann's type analysis

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Abstract

A system of fractional evolution equations results from employing the tool of the Fractional Calculus and following the method used by Dirac to obtain his well-known equation from the Klein-Gordon's one. It represents a possible interpolation between the Dirac and the diffusion equations in one space dimension.

In this paper some analytical properties typical of the general solution of this system of equations are obtained and necessary stability bounds for a numerical scheme approximating such equations are found, through the classical discrete Von Neumann's type analysis.

The non local property of the time fractional differential operator leads to discretizations in terms of series. Here, the analytical methods, usually employed in the study of the stability of discrete schemes when dealing with integer order differential equations, have been adapted to the complexity of the real order case.

Key words: fractional derivatives and integrals, special functions, finite difference methods, stability of numerical methods

1991 MSC: 26A33, 45K05, 65M06, 65M12, 33E12, 35Q40

1 Introduction

The Fractional Calculus (see [3], [13] and [14], for example) deals with the theory of real (or imaginary) order integral and differential operators and it

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represents a natural instrument to model nonlocal phenomena, either in space or time, involving different scales.

The general fractional derivative in the variable x can be denoted by D_x^α , where $\alpha > 0$, and it is asked to coincide with classical derivatives for integer orders α . Many different definitions have been proposed in the literature, preserving this property. Here, we will employ two of the most used ones, in the mathematical and physical fields, respectively.

The first one is the Riemann-Liouville fractional derivative of order $\alpha > 0$ (see [14], for example) of a function f given in $[a, b]$, where $[a, b] \subset \mathbb{R}$, $n \in \mathbb{N}$, $n = -[-\alpha]$ and $x > a$:

$$({}^{RL}_a D_x^\alpha f)(x) = \frac{d^n}{dx^n} \frac{1}{\Gamma(n - \alpha)} \int_a^x \frac{f(\tau)}{(x - \tau)^{\alpha - n + 1}} d\tau. \quad (1)$$

The second one is the Caputo fractional derivative, which can be considered as a regularised version of the previous definition, since it takes the form

$$({}^C_a D_x^\alpha f)(x) = \frac{1}{\Gamma(n - \alpha)} \int_a^x \frac{f^n(\tau)}{(x - \tau)^{\alpha - n + 1}} d\tau. \quad (2)$$

The following relation between the above definitions holds

$$({}^C_a D_x^\alpha f)(x) = {}^{RL}_a D_x^\alpha \left[f(x) - \sum_{j=0}^{n-1} f^{(j)}(a+) \frac{(x - a)^j}{j!} \right], \quad (3)$$

and a sufficient condition under which both derivatives exist is $f \in AC^{n-1}(a, b)$ and $f^n(x) \in L_1[a, b]$. Equivalence (3) allows to include pure initial conditions of the classical type when dealing with fractional equations involving Riemann-Liouville or Caputo derivatives.

In this paper, we consider a generalization of the linear one-dimensional diffusion and wave equations, that we call “fractional evolution Dirac-like equations”. They are obtained by combining the fractional derivatives and the internal degrees of freedom associated to a system, as we explain below.

As a matter of fact, the free Dirac equation is, in some sense, the square root of the Klein-Gordon equation (see, for instance, [16]). Similarly, we can consider a kind of square root of the following fractional diffusion equation in one space dimension:

$$(D_t^{2\alpha} u)(t, x) - \lambda^2 \partial_{xx} u(t, x) = 0, \quad (4)$$

which has been widely studied in the literature (see [6], [7], [8], [9] and [15], for example).

At this purpose, let us consider the general system of fractional evolution Dirac-like equations

$$(\mathbf{A}D_t^\alpha + \lambda\mathbf{B}\partial_x)\mathbf{v}(t, x) = \mathbf{0}, \quad \mathbf{v}(t, x) = \begin{pmatrix} u_1(t, x) \\ u_2(t, x) \end{pmatrix}, \quad (5)$$

with $0 < \alpha \leq 1$, $\lambda \in \mathbb{R}$, $\lambda \neq 0$ and where \mathbf{A} and \mathbf{B} are 2×2 matrixes satisfying the Pauli's algebra:

$$\mathbf{A}^2 = \mathbf{I}, \quad \mathbf{B}^2 = -\mathbf{I}, \quad \mathbf{AB} + \mathbf{BA} = \mathbf{0}. \quad (6)$$

and \mathbf{I} is the identity matrix.

Each component of the solution $\mathbf{v}(t, x)$ also solves (4) provided the index property

$$(D_t^\alpha D_t^\alpha)\mathbf{v}(t, x) = D_t^{2\alpha}\mathbf{v}(t, x) \quad (7)$$

holds (observe that (7) occurs when $\mathbf{v}(0, x) = \mathbf{0}$).

In fact, under the assumption (7), it turns out that:

$$\begin{aligned} (\mathbf{A}D_t^\alpha + \lambda\mathbf{B}\partial_x)\mathbf{v}(t, x) = \mathbf{0} &\implies \\ (\mathbf{A}D_t^\alpha + \lambda\mathbf{B}\partial_x)^2\mathbf{v}(t, x) &= \begin{cases} (D_t^{2\alpha}u_1)(t, x) - \lambda^2\partial_{xx}u_1(t, x) = 0 \\ (D_t^{2\alpha}u_2)(t, x) - \lambda^2\partial_{xx}u_2(t, x) = 0 \end{cases} \end{aligned} \quad (8)$$

Thus, when $1/2 < \alpha < 1$, system (5) represents a fractional interpolation between diffusion ($\alpha = 1/2$) and wave ($\alpha = 1$) equations.

Solutions of this system could model the diffusion of particles whose behavior depends on the space and time coordinates, as usual, but also on their internal structures.

The first formulation involving the mathematical operation of semi-differentiation in replacement of the Fick's law appeared in a work of 1970 by Oldham and Spanier [10]. Later, system (5) was studied by Vázquez et al. ([19], [21], [4] and [11]).

To attribute physical meaning to system (5), we will focus our study on pure real matrixes of Pauli's type leading to non equivalent systems (5). Just two pairs of matrixes fulfill these requirements:

$$\mathbf{A}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{B}_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad (9)$$

$$\mathbf{A}_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathbf{B}_2 = \mathbf{B}_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (10)$$

The first pair (9) reduces system (5) to the following equations of uncoupled variables u_1 and u_2 :

$$(D_t^\alpha u_1)(t, x) - \lambda \partial_x u_1(t, x) = 0, \quad (11)$$

$$(D_t^\alpha u_2)(t, x) + \lambda \partial_x u_2(t, x) = 0. \quad (12)$$

The second pair (10) leads to the system of coupled variables u_1^* and u_2^* :

$$(D_t^\alpha u_1^*)(t, x) + \lambda \partial_x u_2^*(t, x) = 0, \quad (13)$$

$$(D_t^\alpha u_2^*)(t, x) + \lambda \partial_x u_1^*(t, x) = 0. \quad (14)$$

Section 2 of this paper is devoted to show that solutions u_1^* and u_2^* of (13) and (14) can be obtained as a linear combination of u_1 and u_2 , solutions of (11) and (12). This allows to study the general real system (5) just under its specific simple form given by equations (11) and (12).

In Section 3, we search for stability bounds of a numerical scheme approximating the specific fractional evolution-diffusion equation

$$({}_0^C D_t^\alpha u)(t, x) + \lambda \partial_x u(t, x) = 0, \quad (15)$$

in the domain $x > a$, $t > 0$ and together with initial and boundary conditions

$$u(0+, x) = u_0(x), \quad x > a, \quad (16)$$

$$u(t, a+) = r(t), \quad t > 0, \quad (17)$$

where $a \in \mathbb{R}$, $u_0(x)$ and $r(t)$ are known functions, and ${}_0^C D_t^\alpha$ is the Caputo fractional derivative of order α , with $0 < \alpha \leq 1$.

In the literature, numerical formulas approximating fractional derivatives are typically obtained for the Riemann-Liouville expression.

Here, we employ a convolution quadrature formula proposed by Diethelm [1] to approximate the Caputo time fractional derivative and an usual finite difference formula for the space partial derivative. Then, the stability bounds of this scheme are obtained by means of a discrete Von Neumann's type analysis.

These bounds are confirmed by a dispersion-dissipation study in Section 4, and they are finally checked in Section 5 for some representative examples, when we know the underlying exact analytical results.

As far as we know, these techniques have not previously appeared in the literature to analyze a discretization of a fractional differential equation. They represent a fundamental tool in the study of the stability of a numerical scheme; so it could be very useful to know how to adapt them to this non local case.

Finally, as a general remark, it should be highlighted that the idea of considering the square root (or even different order of the roots, as cubic, for instance [19,21]) of a differential equation can be extended to any integer order of such an equation. This allows to study lots of the equations appearing in applied fields from an “internal point of view”, providing therefore an additional information on the associated phenomena.

2 Uncoupled and Coupled Solutions of the System of Fractional Evolution-Diffusion Dirac-like equations

In this section we find the relation existing between the coupled solutions of equations (13) and (14), denoted by u_1^* and u_2^* , and the uncoupled solutions u_1 and u_2 of equations (11) and (12).

Theorem 1 *Let u_1 be the solution of (11) and u_2 the solution of (12). Then:*

$$u_1^* = \frac{u_1 + u_2}{2}, \quad (18)$$

$$u_2^* = \frac{u_2 - u_1}{2}, \quad (19)$$

solve, respectively, equations (13) and (14).

Proof. Let $\mathbf{v}(t, x)$ be the solution of

$$\mathbf{A}_1 D_t^\alpha \mathbf{v}(t, x) + \lambda \mathbf{B}_1 \partial_x \mathbf{v}(t, x) = \mathbf{0}. \quad (20)$$

Then, we want to find two matrixes

$$\mathbf{M} = \begin{pmatrix} m_1 & m_2 \\ m_3 & m_4 \end{pmatrix}, \quad \mathbf{N} = \begin{pmatrix} n_1 & n_2 \\ n_3 & n_4 \end{pmatrix}$$

such that

$$\mathbf{M} \mathbf{A}_1 \mathbf{N} = \mathbf{A}_2, \quad \mathbf{M} \mathbf{B}_1 \mathbf{N} = \mathbf{B}_2. \quad (21)$$

After few calculations, it is found that conditions (21) imply $m_1 = -m_3$, $m_2 = m_4$ and $n_1 = -n_2 = \frac{1}{2m_2}$, $n_3 = n_4 = \frac{1}{2m_1}$. This is:

$$\mathbf{M} = \begin{pmatrix} m_1 & m_2 \\ -m_1 & m_2 \end{pmatrix}, \quad \mathbf{N} = \frac{1}{2} \begin{pmatrix} 1/m_2 & -1/m_2 \\ 1/m_1 & 1/m_1 \end{pmatrix}.$$

On the other hand, solution $\mathbf{v}^*(t, x)$ of (22) has to verify

$$\mathbf{A}_2 D_t^\alpha \mathbf{v}^*(t, x) + \lambda \mathbf{B}_2 \partial_x \mathbf{v}^*(t, x) = \mathbf{0}, \quad \mathbf{v}^*(t, x) = \begin{pmatrix} u_1^*(t, x) \\ u_2^*(t, x) \end{pmatrix}, \quad (22)$$

and, due to (21), it also has to fulfill

$$\mathbf{A}_1 \mathbf{N} D_t^\alpha \mathbf{v}^*(t, x) + \lambda \mathbf{B}_1 \mathbf{N} \partial_x \mathbf{v}^*(t, x) = \mathbf{0}.$$

Therefore, $\mathbf{v}^*(t, x)$ is a solution of (22) if

$$\frac{1}{2m_1} (D_t^\alpha (u_1^*(t, x) + u_2^*(t, x)) + \lambda \partial_x (u_1^*(t, x) + u_2^*(t, x))) = 0, \quad (23)$$

$$\frac{1}{2m_2} (D_t^\alpha (u_1^*(t, x) - u_2^*(t, x)) - \lambda \partial_x (u_1^*(t, x) - u_2^*(t, x))) = 0. \quad (24)$$

It is now straightforward to see that both equations (23) and (24) hold true if u_1^* and u_2^* are given by relations (18) and (19). ■

We conclude this section observing that the results included in Theorem 1 are independent from the definition of the fractional derivative operator appearing in the equations. Also, it should be emphasized that formulas (18) and (19) are still valid whenever one considers the kind of square root of an equation *of any order* by means of the Pauli's matrixes, as we did above.

3 Construction of the numerical scheme

The most important feature of a fractional derivative that has to be taken into account when constructing a numerical scheme is its non-local property. This characteristic leads to discretizations consisting of a lower triangular matrix instead of a multi-diagonal matrix, as in the case of integer order classical derivatives.

In fact, if we suppose $t \in [0, T]$, $x \in [a, b]$, and we introduce the temporal nodes $t_n = n\Delta t$, where $n = 0, \dots, N$, $t_0 = 0$, $t_N = T$, and the spatial nodes $x_l = a + l\Delta x$ where $l = 0, \dots, M$, $x_0 = a$ and $x_M = b$, then the Riemann-Liouville fractional derivative can be approximated as follows

$$\begin{pmatrix} ({}^{RL}D_t^\alpha u)(t_0, x) \\ ({}^{RL}D_t^\alpha u)(t_1, x) \\ \vdots \\ ({}^{RL}D_t^\alpha u)(t_N, x) \end{pmatrix} \approx \frac{1}{\Delta t^\alpha} \begin{pmatrix} \omega_{0,0} & 0 & \cdots & \cdots & 0 \\ \omega_{1,0} & \omega_{1,1} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \omega_{N,0} & \cdots & \cdots & \omega_{N,N} \end{pmatrix} \begin{pmatrix} u(t_0, x) \\ u(t_1, x) \\ \vdots \\ u(t_N, x) \end{pmatrix}.$$

Here we write Δt^α instead of $(\Delta t)^\alpha$ for simplicity.

In an equivalent form, the value of the Riemann-Liouville derivative for each time-space point (t_n, x_l) can be approximated by

$$({}^{RL}D_{t_n}^\alpha u)(t_n, x_l) \approx \frac{1}{\Delta t^\alpha} \sum_{j=0}^n \omega_{n,j} u_l^j, \quad (25)$$

where u_l^n is the numerical approximation of $u(t_n, x_l)$ and it results $u_0^n = u(t_n, a) = r(t_n)$ and $u_l^0 = u(0, x_l) = u_0(x_l)$.

Due to (3), the corresponding approximation for the Caputo derivative is

$$({}^CD_{t_n}^\alpha u)(t_n, x_l) \approx \frac{1}{\Delta t^\alpha} \sum_{j=0}^n \omega_{n,j} u_l^j - \frac{t_n^{-\alpha} u_0(x_l)}{\Gamma(1-\alpha)}. \quad (26)$$

In this paper we employ the convolution quadrature formula (25) with the weights $\omega_{n,j}$ proposed by Diethelm in [1]:

$$\Gamma(2-\alpha)\omega_{n,j} = \begin{cases} 1 & j = n \\ (n-j-1)^{1-\alpha} - 2(n-j)^{1-\alpha} + (n-j+1)^{1-\alpha} & 1 \leq j \leq n-1 \\ (n-1)^{1-\alpha} - (\alpha-1)n^{-\alpha} - n^{1-\alpha} & j = 0 \end{cases} \quad (27)$$

It has been shown [1] that the convergence order associated to this formula is $O(\Delta t)^{2-\alpha}$.

As well, the weights obtained by Lubich in [5] by means of the so called *discretized operational calculus* could have been used instead of the ones given in (27). However, such weights lead to an approximation for the Riemann-Liouville derivative with a convergence order $O(\Delta t)^\alpha$. So, as in our

case the index of the fractional derivative in time varies between 0 and 1, Diethelm's weights turn out to be advantageous.

In combination with the discrete formula (25) involving Diethelm's weights for the time fractional derivative, we employ a classical forward Euler formula to approximate the first order space derivative:

$$\partial_x u(t_n, x_l) \approx \frac{u_{l+1}^n - u_l^n}{\Delta x}. \quad (28)$$

Now, if we write the fractional evolution-diffusion equation (15) by means of the following integral equation with a strongly singular kernel

$$\frac{1}{\Gamma(-\alpha)} \int_0^t \frac{u(\tau, x)}{(t - \tau)^{\alpha+1}} d\tau - \frac{t^{-\alpha} u_0(x)}{\Gamma(1 - \alpha)} + \lambda \partial_x u(t, x) = 0, \quad (29)$$

and we use formula (25) with weights (27) instead of the time fractional derivative and formula (28) for the space derivative, then the finite difference equation corresponding to (29) is:

$$u_{l+1}^n = \left(1 - \omega_{n,n} \frac{\Delta x}{\lambda \Delta t^\alpha}\right) u_l^n + \frac{\Delta x}{\lambda} \left[\frac{u_0(x_l) t_n^{-\alpha}}{\Gamma(1 - \alpha)} - \sum_{j=0}^{n-1} \frac{\omega_{n,j}}{\Delta t^\alpha} u_l^j \right], \quad (30)$$

for all $l = 0, \dots, M - 1$ and $n = 1, \dots, N$. It is straightforward to see that the error associated to formula (30) is $O(\Delta t)^{2-\alpha} + O(\Delta x)$.

Now then, let us present the main result on the stability obtained from the discrete Von Neumann's type analysis of the scheme (30) together with initial condition (16).

Theorem 2 *Given the numerical scheme (30) approximating the fractional evolution equation (15) together with the initial condition (16), a necessary condition for the scheme to be stable for all $\alpha \in (0, 1)$ is:*

$$\frac{\Delta x}{\lambda \Delta t^\alpha \Gamma(2 - \alpha)} \leq 1. \quad (31)$$

Proof. Let us introduce in equation (30) the discrete Fourier mode

$$u_l^n = \tau^n e^{ilQ\Delta x}, \quad (32)$$

where it is assumed $Q = m\pi$, being m an integer such that $0 \leq m \leq M$, and the super index of τ stands for its n -th power. Then, after dividing by $e^{ilQ\Delta x}$, it results

$$\tau^n \left(e^{iQ\Delta x} - 1 + \frac{\Delta x}{\lambda \Delta t^\alpha \Gamma(2 - \alpha)} \right) = - \sum_{j=0}^{n-1} \bar{\omega}_{n,j} \tau^j \quad (33)$$

where

$$\bar{\omega}_{n,j} = \begin{cases} -\frac{\Delta x((n-j)^{1-\alpha} - (n-j-1)^{1-\alpha} - ((n-j+1)^{1-\alpha} - (n-j)^{1-\alpha}))}{\lambda \Delta t^\alpha \Gamma(2-\alpha)} & j = 1, \dots, n-1 \\ -\frac{\Delta x(n^{1-\alpha} - (n-1)^{1-\alpha})}{\lambda \Delta t^\alpha \Gamma(2-\alpha)} & j = 0 \end{cases}. \quad (34)$$

Therefore, if we assume

$$L = \left(e^{iQ\Delta x} - 1 + \frac{\Delta x}{\lambda \Delta t^\alpha \Gamma(2-\alpha)} \right), \quad (35)$$

the key idea is to rewrite (33) through the following equivalent expression:

$$\tau^n = -\frac{\bar{\omega}_{n,0}}{L} \prod_{j=1}^{n-1} \left(1 - \frac{\bar{\omega}_{n,j}}{L} \right). \quad (36)$$

So, if we use the notation

$$A_\alpha = \frac{\Delta x}{\lambda \Delta t^\alpha \Gamma(2-\alpha)}, \quad (37)$$

it results:

$$|1 - |1 - A_\alpha|| \leq |L = L(Q)| \leq 1 + |1 - A_\alpha|, \quad \forall Q. \quad (38)$$

Then

$$|\tau(Q)|^n \leq \frac{|A_\alpha| z(n, \alpha)}{|1 - |1 - A_\alpha||} \prod_{j=1}^{n-1} \left(1 + \frac{|A_\alpha| s(j, \alpha)}{|1 - |1 - A_\alpha||} \right) \quad \forall Q, \quad n \geq 2, \quad (39)$$

where

$$z(n, \alpha) = (n^{1-\alpha} - (n-1)^{1-\alpha}), \quad (40)$$

$$s(j, \alpha) = (n-j)^{1-\alpha} - (n-j-1)^{1-\alpha} - ((n-j+1)^{1-\alpha} - (n-j)^{1-\alpha}); \quad (41)$$

when $n = 1$,

$$|\tau(Q)| \leq \frac{|A_\alpha|}{|1 - |1 - A_\alpha||} \quad \forall Q. \quad (42)$$

Observe that, due to the non negativity and the decreasing character of $z(n, \alpha)$ with respect to n for all $0 < \alpha < 1$, also function $s(j, \alpha)$ turns out to be non negative for all $j = 1, \dots, n-1$ and $0 < \alpha < 1$. In fact, these two functions are non negative for all $0 \leq \alpha \leq 1$.

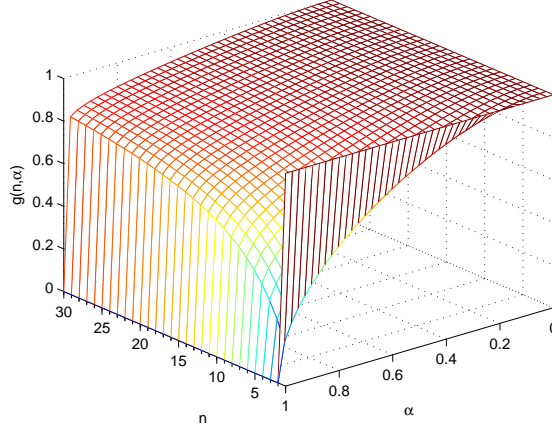


Fig. 1. Function $g(n, \alpha)$ for different values of n and α

Therefore, if we assume that $\prod_{j=1}^0 \left(1 + \frac{|A_\alpha|s(j, \alpha)}{|1 - |A_\alpha||}\right) = 1$, we can separate three possible cases:

- if $A_\alpha < 1$

$$|\tau(Q)|^n \leq z(n, \alpha) \prod_{j=1}^{n-1} (1 + s(j, \alpha)), \quad \forall Q, \quad n \geq 1, \quad (43)$$

- if $A_\alpha = 1$

$$|\tau(Q)|^n = z(n, \alpha) \prod_{j=1}^{n-1} (1 + s(j, \alpha)), \quad \forall Q, \quad n \geq 1, \quad (44)$$

- if $A_\alpha > 1$

$$|\tau(Q)|^n \leq \frac{|A_\alpha| z(n, \alpha)}{|2 - A_\alpha|} \prod_{j=1}^{n-1} \left(1 + \frac{|A_\alpha| s(j, \alpha)}{|2 - A_\alpha|}\right), \quad \forall Q, \quad n \geq 1. \quad (45)$$

Note that expression $|A_\alpha| / |2 - A_\alpha|$ appearing in (45) turns out to be bigger than 1 if $A_\alpha > 1$.

Now then, we ask for $|\tau| \leq 1$ for all Q , in order to obtain the necessary condition for the stability of the numerical scheme (30) (see [17], for example).

Our aim is to show that this restriction, called the discrete Von Neumann's criterion, is here equivalent to require $A_\alpha \leq 1$.

To do that, let us consider the following function:

$$g(n, \alpha) = \left(z(n, \alpha) \prod_{j=1}^{n-1} (1 + s(j, \alpha)) \right)^{1/n}, \quad (46)$$

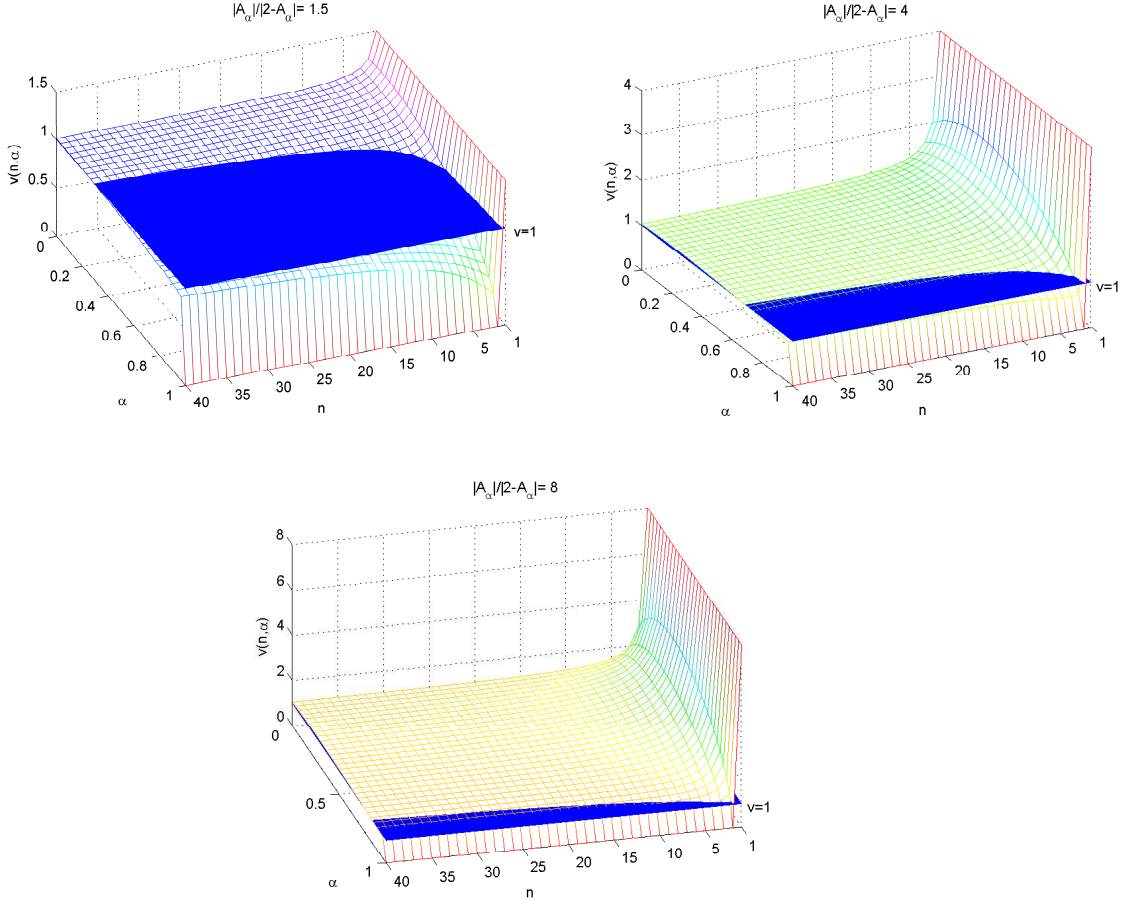


Fig. 2. Function $v(n, \alpha)$ for different values of $|A_\alpha|/|2 - A_\alpha|$: 1.5, 4, 8.

which represents the maximum of $|\tau(Q)|$ with respect to Q in the case $A_\alpha \leq 1$. Then, it has been numerically observed that all the values taken by $g(n, \alpha)$ for different n and α such that $0 \leq \alpha \leq 1$, are always below 1.

As an example, Fig.1 plots $g(n, \alpha)$ for $n = 1, 2, \dots, 30$ and $\alpha = 0, h, 2h, \dots, 1$, with $h = 1/40$.

On the contrary, the function

$$v(n, \alpha) = \left(\frac{|A_\alpha| z(n, \alpha)}{|2 - A_\alpha|} \prod_{j=1}^{n-1} \left(1 + \frac{|A_\alpha| s(j, \alpha)}{|2 - A_\alpha|} \right) \right)^{1/n} \quad (47)$$

appearing in (45) and returning the maximum value of $|\tau(Q)|$ with respect to Q in the case $A_\alpha > 1$, is always above 1 in an interval of values of α which grows as the value of $|A_\alpha|/|2 - A_\alpha|$ increases. To illustrate this assertion, Fig.2 is included, obtained for $n = 1, 2, \dots, 40$, $\alpha = 0, h, 2h, \dots, 1$, $h = 1/30$, and different values of $|A_\alpha|/|2 - A_\alpha|$.

From this, it can be concluded that necessarily condition (31) has to hold, in

order to be $|\tau| \leq 1$ for all Q and α , when $0 < \alpha < 1$. ■

As a remark, it has to be said that (39) returns the classical stability conditions for the limiting cases $\alpha = 0$ and $\alpha = 1$.

In fact, due to (3), the fractional evolution-diffusion equation (15) can be rewritten as follows

$$({}^{RL}D_t^\alpha u)(t, x) - \frac{u_0(x)t^{-\alpha}}{\Gamma(1-\alpha)} + \lambda \partial_x u(t, x) = 0. \quad (48)$$

Then, holding $({}^{RL}D_t^1 u)(t, x) = \partial_t u(t, x)$ and $({}^{RL}D_t^0 u)(t, x) = u(t, x)$, equation (48) is reduced to

$$\partial_t u(t, x) + \lambda \partial_x u(t, x) = 0, \quad (49)$$

when $\alpha = 1$, whereas it is given by equation

$$u(t, x) - u_0(x) + \lambda \partial_x u(t, x) = 0, \quad (50)$$

when $\alpha = 0$.

Now, Diethelm's weights $\omega_{n,j}$ defined in (27) verify, when $\alpha = 1$, that $\omega_{n,j} = 0$ for all $j = 0, 1, \dots, n-2$ and $\omega_{n,n} = 1$, $\omega_{n,n-1} = -1$. As well, when $\alpha = 0$, $\omega_{n,j} = 0$ for all $j = 0, 1, \dots, n-1$ and $\omega_{n,n} = 1$. So, the finite difference equation (30), when $\alpha = 1$, reads

$$u_{l+1}^n = \left(1 - \frac{\Delta x}{\lambda \Delta t}\right) u_l^n + \frac{\Delta x}{\lambda \Delta t} u_l^{n-1}, \quad (51)$$

being $\frac{u_0(x_l)t_n^{-\alpha}}{\Gamma(1-\alpha)}|_{\alpha=1} = 0$, whereas, when $\alpha = 0$, it is the following:

$$u_{l+1}^n = \left(1 - \frac{\Delta x}{\lambda}\right) u_l^n + \frac{\Delta x}{\lambda} u_0(x_l). \quad (52)$$

Schemes (51) and (52) are exactly the which ones we would obtain applying forward Euler formulas to discretize the first order derivatives in space and time appearing in (49), and just the first order space derivative included in (50), respectively.

Von Neumann's type analysis of stability of scheme (51) leads to the following equation for τ :

$$\tau^n \left(e^{iQ\Delta x} - 1 + \frac{\Delta x}{\lambda \Delta t} \right) = \frac{\Delta x}{\lambda \Delta t} \tau^{n-1}, \quad (53)$$

which is equivalent to

$$\tau = \left[\frac{A_1}{(e^{iQ\Delta x} - 1 + A_1)} \right], \quad (54)$$

where $A_1 = \Delta x / (\lambda \Delta t) = A_\alpha|_{\alpha=1}$.

From this, the inequality

$$|\tau(Q)| \leq \frac{|A_1|}{|1 - |1 - A_1||}, \quad \forall Q, \quad (55)$$

is deduced and therefore it results:

- if $A_1 < 1$

$$|\tau(Q)| \leq 1, \quad \forall Q, \quad (56)$$

- if $A_1 = 1$

$$|\tau(Q)| = 1, \quad \forall Q, \quad (57)$$

- if $A_1 > 1$

$$|\tau(Q)| \leq \frac{|A_1|}{|2 - A_1|}, \quad \forall Q. \quad (58)$$

Then, according to the Von Neumann's criterion, a necessary condition for the stability of scheme (51) is $A_1 = \Delta x / (\lambda \Delta t) \leq 1$.

As it was to be expected, inequality (55) can be obtained from (39) since the function $z(n, \alpha)$ defined in (40) verifies $z(n, 1) = 1$ if $n = 1$ and $z(n, 1) = 0$ if $n \geq 2$. As well, looking at Fig.1, it can be seen that when $A_\alpha \leq 1$, the function

$$g(n, \alpha) = \max_{Q=0, \pi, \dots, M\pi} |\tau(Q)|$$

corresponding to $\alpha = 1$ is equal to 1 when $n = 1$ and to 0 when $n \geq 2$.

In addition to that, Fig.2 also shows that, when $A_\alpha > 1$, function

$$v(n, \alpha) = \max_{Q=0, \pi, \dots, M\pi} |\tau(Q)|$$

is equal to $|A_\alpha| / |2 - A_\alpha|$ if $\alpha = 1$.

On the other hand, when $\alpha = 0$ the discrete Von Neumann's analysis of stability for the scheme (51) leads to the following equation for τ :

$$\tau^n \left(e^{iQ\Delta x} - 1 + \frac{\Delta x}{\lambda} \right) = \frac{\Delta x}{\lambda} \quad (59)$$

which is equivalent to

$$\tau = \left[\frac{A_0}{(e^{iQ\Delta x} - 1 + A_0)} \right]^{1/n}, \quad (60)$$

where $A_0 = \Delta x / \lambda = A_\alpha|_{\alpha=0}$.

So, the following inequality can be written:

$$|\tau(Q)| \leq \left[\frac{|A_0|}{|1 - |1 - A_0||} \right]^{1/n}, \quad \forall Q, \quad (61)$$

which implies:

- if $A_0 < 1$

$$|\tau(Q)| \leq 1, \quad \forall Q, \quad (62)$$

- if $A_0 = 1$

$$|\tau(Q)| = 1, \quad \forall Q, \quad (63)$$

- if $A_0 > 1$

$$|\tau(Q)| \leq \left[\frac{|A_0|}{|2 - A_0|} \right]^{1/n}, \quad \forall Q. \quad (64)$$

Once again, the necessary condition of stability for the scheme (52) is obtained by imposing $|\tau| \leq 1$, that leads to $A_0 = \Delta x / \lambda \leq 1$.

As for the case $\alpha = 1$, inequality (39) returns (61) when $\alpha = 0$ due to the fact that $z(n, \alpha)$ verifies $z(n, 0) = 1$ for all $n \geq 1$, whereas $s(n, \alpha)$, defined for $n \geq 2$, fulfills $s(j, 0) = 0$ for all $j = 1, \dots, n - 1$.

As well, Fig.1 shows that, when $A_\alpha \leq 1$, function

$$g(n, \alpha) = \max_{Q=0, \pi, \dots, M\pi} |\tau(Q)|$$

equals 1 for all n in correspondence of $\alpha = 0$, according to results (62) and (63). This means that $\max_{Q=0, \pi, \dots, M\pi} |\tau(Q)| = 1$ when $A_0 \leq 1$.

Also, when $A_\alpha > 1$, the function

$$v(n, \alpha) = \max_{Q=0, \pi, \dots, M\pi} |\tau(Q)|$$

takes the value $(|A_\alpha| / |2 - A_\alpha|)^{1/n}$ if $\alpha = 0$, in accordance with inequality (64) from which relation

$$\max_{Q=0, \pi, \dots, M\pi} |\tau(Q)| = (|A_0| / |2 - A_0|)^{1/n}$$

is deduced when $A_0 > 1$, and also in agreement with the graphics appearing in Fig.2.

4 Dispersion-dissipation relation

4.1 Motivation

Usually, while solving analytically a partial differential equation, the dispersion-dissipation relation $\omega = \omega(\beta)$ [20] is pursued so that the following wave in time and space

$$u(t, x) = \hat{u} e^{i(\omega t + \beta x)} \quad (65)$$

is a solution of such an equation (see [17], for instance).

If we consider the parabolic diffusion equation

$$\partial_t u(t, x) - \nu \partial_{xx} u(t, x) = 0, \quad (66)$$

and the hyperbolic evolution equation

$$\partial_t u(t, x) + \lambda \partial_x u(t, x) = 0, \quad (67)$$

then the function (65) solves equation (66) if $\omega = i\nu\beta^2$, and it solves equation (67) while $\omega = -\lambda\beta$.

Therefore, the wave solving (66) takes the form

$$u(t, x) = \hat{u} e^{-\nu\beta^2 t} e^{i\beta x}, \quad (68)$$

and it does not move in space whereas it decays in time if $\nu > 0$. This is the typical behavior shown by wave solutions of parabolic type equations.

As well, solution (65) of equation (67) takes the expression

$$u(t, x) = \hat{u} e^{i\beta(x - \lambda t)}, \quad (69)$$

which is a wave propagating along the x axe with a speed $\lambda = -\omega/\beta$ and without any decay in the amplitude. In particular, when ω is a linear function of β , the propagation speed is independent from the frequency.

Decay and propagation of the different Fourier modes are very important to describe the behavior of the solution of a partial differential equation.

In fact, solutions of partial differential equations are said to be *dissipative* when the Fourier modes do not grow in time and one, at least, decays. This is the case, for example, of the solutions (68) of the diffusion equation (66), which all dissipate when $\nu > 0$, except for the constant solution $u(t, x) = \hat{u}$ associated to the wave number $\beta = 0$, that is not well determined by equation (66). Solutions are said to be *non dissipative* when the Fourier modes do not

grow nor decay, as it occurs with the waves (69) solving the evolution equation (67).

Finally, solutions of partial differential equations are said to be *dispersive* if the Fourier modes having different wavelengths propagate with different speeds; this is the case, for example, of the solutions of equations just involving partial derivative in x of order equal or bigger than 1.

On the other side, when a finite difference equation is employed to approximate the continuous solution of a partial differential equation, the behavior of its numerical solution also depends on if the discrete Fourier modes decay or grow. For example, it can be said that the numerical scheme is unstable whenever some modes grow without bounds.

4.2 The fractional case

In the particular case under study in this section, the wave function (65) has to be a solution of the fractional evolution-diffusion Dirac like equation (15). Then we obtain a dispersion-dissipation relation much more complex than the which ones appearing in the examples above.

In fact, in view of the property (3) and the following:

$$({}^{RL}D_x^\alpha u)e^{\lambda x} = \frac{e^{\lambda a}}{(x-a)^\alpha} E_{1,1-\alpha}(\lambda x - \lambda a) \quad (70)$$

where $\lambda \in \mathbb{R}$ and the definition of the Mittag-Leffler function [2] is

$$E_{\alpha,\beta}(z) = \sum_{j=0}^{\infty} \frac{z^j}{\Gamma(\alpha j + \beta)} = \frac{1}{2\pi i} \int_{Ha} \frac{e^\sigma \sigma^{\alpha-\beta}}{\sigma^\alpha - z} d\sigma, \quad (71)$$

being $\{\alpha, \beta, z\} \in \mathbb{C}$, $\text{Re}(\alpha) > 0$, we have:

$$\begin{aligned} {}^C D_t^\alpha \hat{u} e^{i(\omega t + \beta x)} &= \hat{u} t^{-\alpha} e^{i\beta x} E_{1,1-\alpha}(i\omega t) - \hat{u} \frac{t^{-\alpha}}{\Gamma(1-\alpha)} e^{i\beta x} = \\ &= i\omega \hat{u} t^{1-\alpha} e^{i\beta x} E_{1,2-\alpha}(i\omega t). \end{aligned}$$

So, the dispersion-dissipation relation associated to equation (15) is given by the following expression:

$$\omega t^{1-\alpha} E_{1,2-\alpha}(i\omega t) = -\lambda \beta e^{i\omega t}. \quad (72)$$

When $\alpha = 1$, formula (72) coincides with the relation obtained for the evolution equation (67). When $\alpha \neq 1$, it is not possible to obtain explicitly ω as

a function of β . It results, in fact, $\omega = \omega(\beta, t)$ due to the non local character of the fractional differential operator. As a consequence, the dispersion-dissipation relation also involves time.

Now, keep on considering the behavior of the Fourier modes solving the numerical scheme (30) associated to equation (67).

The first step is to provide the discrete analogous of the Fourier mode (65):

$$u_l^n = \hat{u} e^{i\omega n \Delta t} e^{il\beta \Delta x}. \quad (73)$$

Then, as in the continuous case, we search for the relation $\omega = \omega(\beta)$ allowing (73) to be a solution of (30).

According to the calculations we realized in the proof of Theorem 2, and particularly result (36), we can write

$$e^{i\omega \Delta t} = -\frac{\bar{\omega}_{1,0}}{(e^{i\beta \Delta x} - 1 + A_\alpha)} = \frac{A_\alpha}{(e^{i\beta \Delta x} - 1 + A_\alpha)} = \frac{A_\alpha}{L}. \quad (74)$$

Here: the weight $\bar{\omega}_{1,0}$ is deduced from (34), the expressions for A_α and L have been given in (37) and (35), respectively, provided Q is substituted by β .

Now, if we write $\omega = a + ib$, it turns out to be $e^{i\omega \Delta t} = e^{ia\Delta t} e^{-b\Delta t}$, where

$$b = -\frac{1}{\Delta t} \ln \frac{|A_\alpha|}{|L|}. \quad (75)$$

Consequently, all the waves given by (73) with $\beta \neq 0$ decay if $b > 0$, that means if $\frac{|A_\alpha|}{|L|} < 1$, and this is fulfilled if $A_\alpha = \frac{\Delta x}{\lambda \Delta t^\alpha \Gamma(2-\alpha)} < 1$. Therefore, under this restriction the scheme is dissipative and a necessary condition for the scheme to be stable is found. Note that, this is exactly the necessary condition (31) provided in Theorem 2. If $\beta = 0$, the Fourier mode (73) does not grow nor decay and the scheme is not dissipative. Finally, when $\beta \neq 0$ and $b < 0$, the scheme is unstable because some Fourier modes are unbounded.

On the other side, it turns out to be

$$e^{ia\Delta t} = \frac{A_\alpha}{L} \frac{|L|}{|A_\alpha|} = \frac{A_\alpha}{|A_\alpha|} (\cos(\beta \Delta x) + A_\alpha - 1 - i \sin(\beta \Delta x)), \quad (76)$$

and so

$$\tan(a\Delta t) = -\frac{\sin(\beta \Delta x)}{\cos(\beta \Delta x) + A_\alpha - 1}. \quad (77)$$

As a consequence,

$$a = -\frac{1}{\Delta t} \arctan \left(\frac{\sin(\beta \Delta x)}{A_\alpha - 2 \sin^2 \left(\frac{\beta \Delta x}{2} \right)} \right), \quad (78)$$

and the scheme is dispersive, being this expression not a linear function in β .

Generally speaking, when a numerical scheme shows dissipation and dispersion at the same time, then dissipation uses to hide dispersion and the Fourier modes which try to move at a wrong velocity are muffled. If one wanted to confirm this assumption, then he should study both the behavior of $e^{-b\Delta t}$, in order to see how the solution dissipates, and of the error in the propagation speed of the Fourier mode involving $\beta \Delta x$, for all $0 \leq \beta \Delta x \leq \pi$. Said error is the difference between the exact propagation speed of the wave (65) solving (15) (represented by the function of β given by $-\omega/\beta$, that we would know explicitly if we could find the explicit expression of ω as a function of β starting from relation (72)) and the speed of propagation of the discrete Fourier mode (73), given by

$$-a/\beta = \frac{1}{\beta \Delta t} \arctan \left(\frac{\sin \beta \Delta x}{A_\alpha - 2 \sin^2 \frac{\beta \Delta x}{2}} \right),$$

for all $0 \leq \beta \Delta x \leq \pi$.

5 Numerical results

To conclude, we show numerical results emerging from simulations of the evolution-diffusion equation (15) together with the specific initial-boundary conditions

$$u(0+, x) = e^{-\mu x}, \quad x > a, \quad (79)$$

$$u(t, a+) = e^{-\mu a} E_{\alpha,1}(\mu \lambda t^\alpha), \quad t > 0,$$

where $a \in \mathbb{R}$, $\mu > 0$ and $0 < \alpha < 1$. These simulations employed the scheme (30), in order to check the stability bounds (31).

The analytical solution of this problem was obtained in [12] and it is given by

$$u_\alpha(t, x) = e^{-\mu x} E_{\alpha,1}(\mu \lambda t^\alpha), \quad (80)$$

for all $x \geq a$ and $t \geq 0$. According with the properties of the Mittag-Leffler function, it takes the specific forms:

$$u_{1/2}(t, x) = e^{-\mu x} e^{\mu^2 \lambda^2 t} \operatorname{erfc}(-\mu \lambda \sqrt{t}), \quad (81)$$

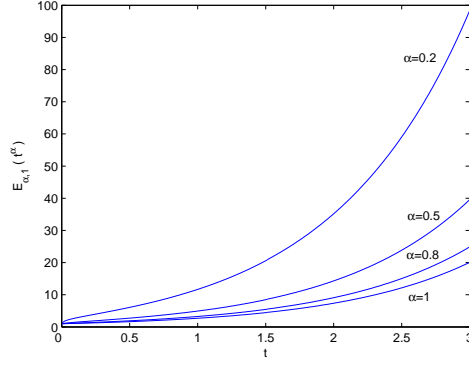


Fig. 3. Function $E_{\alpha,1}(t^\alpha)$ for $0 \leq t \leq 3$ when $\alpha = 0.2$, $\alpha = 0.5$, $\alpha = 0.8$ and $\alpha = 1$

$$u_1(t, x) = e^{-\mu(x-\lambda t)}. \quad (82)$$

In the practice, to provide the values of (80), the Mittag-Leffler serie is calculated by solving numerically the ordinary differential equation

$$({}_0^C D_t^\alpha u)(t) - \mu \lambda u(t) = 0, \quad (83)$$

with the initial condition $u(0) = 1$, being $E_{\alpha,1}(\mu \lambda t^\alpha)$ the exact solution of this problem.

Fig.3 represents the function $E_{\alpha,1}(t^\alpha)$ for $t \in [0, 3]$ and when $\alpha = 0.2$, $\alpha = 0.5$, $\alpha = 0.8$ and $\alpha = 1$.

The software Matlab7.0 working in double precision has been employed to perform all the involved numerical simulations.

An interesting example confirming that condition (31) over time and space steps of the finite difference scheme (30) is necessary in order to have stability, is the following. We calculated the maximum of the absolute errors resulting between the values of the exact solution (80), numerically evaluated over the space-time grid points, and the approximated ones produced by the implementation of the difference scheme (30) when $\mu = \lambda = 1$, $x \in [1, 3.5]$, $\Delta x = 0.025$, $t \in [0, 2]$, $\Delta t = 0.0125$. Then, we observed that its value is 0.1189 when $\alpha = 0.1$, 0.00241 when $\alpha = 0.5$ and that it is unbounded when $\alpha = 0.9$.

The result concerning $\alpha = 0.9$, is due to the breaking of th condition (31). In fact, relation $(\Delta x / (\Delta t^\alpha \Gamma(2 - \alpha))) \leq 1$ comes true if $\alpha = 0.1$ and $\alpha = 0.5$, whereas it is not fulfilled when $\alpha = 0.9$, being $\Delta x = 0.025$, $\Delta t^{0.9} = 0.0194$ and $\Gamma(1.1) = 0.9513$. Now, if we simulate the same solutions when $\mu = 1$, $x \in [1, 3.5]$, $\Delta x = 0.025$, $t \in [0, 2]$, $\Delta t = 0.0125$, but $\lambda = -1$, we find that the scheme (30) converges only when $\alpha = 0.1$ and it diverges for $\alpha = 0.5$ and $\alpha = 0.9$.

The wide number of simulations we performed for different values of α , Δx , Δt and λ , indicates that a necessary and sufficient condition ensuring the stability of the difference scheme (30) should be almost stronger than the pure necessary condition we provided in (31).

To obtain both a necessary and sufficient condition of stability, a discrete generalized Von Neumann analysis should be driven, based, instead than on the usual Fourier mode (32), on some appropriate functions deduce by applying discrete method of separation of variables to the problem under study (see [17, Chapt. 3]). Also, a different method taking boundary conditions into account and leading to stronger conditions of stability is the so called “GKSO”, detailed in [18].

6 Conclusions

The *non local* feature of the integral operators defining real order derivatives is in contrast with the local behavior of the classical integer order differential operators, which can be evaluated considering values of the function under derivation in an arbitrary small interval around the variable. This property of *memory* of the fractional derivatives leads to very complex discretizations of these operators and, as a consequence, the arithmetic cost of the corresponding algorithms increases, with respect to the methods usually employed when dealing with integer order differential equations.

In this paper we constructed a numerical scheme solving the fractional evolution-diffusion equation and we developed the corresponding classical discrete Von Neumann’s type analysis that revealed pure necessary conditions of stability which, in general, are not sufficient. However this was to be expected. Indeed, from a theoretical point of view, when a Von Neumann’s type analysis is carried out on finite difference schemes associated to initial-boundary values problems for parabolic equations, it leads to stability conditions that are both necessary and sufficient if the matrix associated to the scheme is symmetric. When dealing with schemes for hyperbolic equations, as in our case, almost never a symmetric matrix can be expected and so only pure necessary conditions are deduced.

On the other hand, the dispersion-dissipation study for the numerical scheme highlighted that it is dissipative when the necessary condition of stability derived from the Von Neumann’s type analysis is fulfilled. Also, the scheme turned out to be dispersive, although this behavior could not be observed whenever, as it usually occurs, the dissipation hides the dispersion and the Fourier components moving at a wrong velocities are muffled.

In conclusion, the continuous and discrete evolution-diffusion equations of the Dirac's type, representing a generalization of the classical evolution, diffusion and wave equations, show a dispersion-dissipation behavior in the middle between the parabolic (dissipative) and the hyperbolic one (non dissipative). It is very typical, when dealing with fractional operators, to obtain results generalizing and interpolating the classical ones corresponding to integer order cases.

Acknowledgements: The author is grateful to L. Vázquez for fruitful discussions and suggestions concerning the subject of the paper. Also, she acknowledges T. Cazenave and A. Haurox for providing her with all the research facilities at the Laboratoire Jacques-Louis Lions (Paris, France) where the present investigation took shape.

Finally she thanks the partial support of the Ministry of Education and Science of Spain under grant MTM2005-05573 and the financial support from the *Programa de Creación y Consolidación de grupos de investigación. Universidad Complutense-Comunidad de Madrid (Nº910711)*.

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