ANZIAM J. 52(2010), 123–138
doi:10.1017/S1446181111000617

REGULARITY OF SOLUTIONS TO A TIME-FRACTIONAL DIFFUSION EQUATION

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(Received 26 October, 2010; revised 15 March, 2011)

Abstract

We prove estimates for the partial derivatives of the solution to a time-fractional diffusion equation posed over a bounded spatial domain. Such estimates are needed for the analysis of effective numerical methods, particularly since the solution is typically less regular than in the familiar case of classical diffusion.

2000 *Mathematics subject classification*: primary 35B65, secondary 35C15, 35C20.

Keywords and phrases: fractional derivative, Laplace transform, Sobolev space, singular behaviour.

1. Introduction

In classical diffusion, the density $u(x, t)$ of particles at position x and time t obeys the parabolic partial differential equation

$$u_t - \nabla \cdot (K \nabla u) = f, \tag{1.1}$$

where $u_t = \partial u/\partial t$, $f = f(x, t)$ is the density of sources, $K > 0$ is the diffusivity, and ∇u is the spatial gradient of u. In anomalous subdiffusion, u instead satisfies the partial integro-differential equation

$$u_t - \nabla \cdot (\omega_\nu * K \nabla u)_t = f, \tag{1.2}$$

with $0 < \nu < 1$, where $\omega_\nu(t) = t^{\nu-1}/\Gamma(\nu)$ and $*$ denotes the Laplace convolution. Our aim is to describe the smoothness, or lack thereof, of solutions to (1.2).

We can interpret the parameter ν at the microscopic level [6, 12]: the diffusing particles have a mean-square displacement $2Kt^\nu/\Gamma(1 + \nu) \propto t^\nu$. For example, Golding and Cox [3] tracked the motion of RNA molecules inside live *E. coli* cells and observed subdiffusion with an exponent $\nu = 0.7 \pm 0.07$. By contrast, in the classical setting of Brownian motion the mean-square displacement is $2Kt$, for which the exponent takes the limiting value $\nu = 1$.

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For any $\mu > 0$, the convolution

$$(\omega_\mu * w)(t) = \int_0^t \frac{(t-s)^{\mu-1}}{\Gamma(\mu)} w(s)\,ds$$

defines the Riemann–Liouville fractional integral of w of order μ, and we may interpret $(\omega_\nu * w)_t$ as the fractional *derivative* $\partial_t^{1-\nu} w$. If $\nu \to 1$ then $(\omega_\nu * w)_t \to w$ and we recover the classical diffusion equation (1.1) as a limiting case of (1.2).

For a bounded domain $\Omega \subseteq \mathbb{R}^d$ with spatial dimension $d \geq 1$, we impose homogenous boundary conditions, either of Dirichlet (absorbing) type,

$$u(x,t) = 0 \quad \text{for } x \in \partial\Omega \text{ and } t > 0, \tag{1.3}$$

or else of Neumann (reflecting) type,

$$\partial_n u(x,t) = 0 \quad \text{for } x \in \partial\Omega \text{ and } t > 0, \tag{1.4}$$

where n denotes the outward unit normal to Ω. We also assume the initial condition

$$u(x,0) = u_0(x) \quad \text{for } x \in \Omega.$$

It is convenient to define the second-order, self-adjoint, elliptic partial differential operator $Au = -\nabla \cdot (K\nabla u)$, and to rewrite (1.2) as

$$u_t + (\omega_\nu * Au)_t = f(t). \tag{1.5}$$

An understanding of the regularity of u is crucial for the design of effective numerical methods for (1.5), especially since u is typically less regular than in the classical case. For a simple example, let $f \equiv 0$ and $u_0 = \phi$, where ϕ is an eigenfunction of A, say $A\phi = \lambda\phi$. It follows from (2.4) and (2.6) below that

$$u(x,t) = \phi(x)\Big(1 - \frac{\lambda t^\nu}{\Gamma(1+\nu)} + O(t^{2\nu})\Big) \quad \text{as } t \to 0.$$

So, since $0 < \nu < 1$, the derivatives of u with respect to t are unbounded as $t \to 0$.

The motivation for this paper came from an analysis of discontinuous Galerkin methods [9, 14], which assumed regularity estimates of the form

$$t^\nu \|Au'(t)\| + t^{1+\nu}\|Au''(t)\| + t^{2+\nu}\|Au'''(t)\| \leq Ct^{\sigma-1} \tag{1.6}$$

and

$$\|u'(t)\| + t\|u''(t)\| \leq Ct^{\sigma-1}, \tag{1.7}$$

for $0 < t \leq T$, with $\sigma > 0$ and C a generic, positive constant. We establish such estimates in Theorems 4.4 and 5.7.

In Section 2, we solve the initial boundary value problem for (1.2) using separation of variables and Laplace transformation. This construction is standard [5, 13] so we merely outline the main steps, introducing our notation in the process. Section 3 summarizes some key facts concerning the function space $\dot{H}^r \subseteq H^r(\Omega)$ that we use to measure the spatial regularity of u.

Having dealt with these preliminaries, in Section 4 we suppose that $f \equiv 0$ and prove bounds of the form

$$t^q \|u^{(q)}(t)\|_{\dot{H}^{r+\mu}} \leq Ct^{-\mu\nu/2}\|u_0\|_{\dot{H}^r}, \tag{1.8}$$

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for $q \in \{1, 2, 3, \ldots\}$ and $0 \le r < \infty$. Here the additional smoothing in space is limited to $0 \le \mu \le 2$, in contrast to the classical case $\nu = 1$ where μ may be arbitrarily large. The method of proof was used previously [8, 10] to deal with a fractional *wave* equation, corresponding to the case $1 < \nu < 2$. We also obtain an expansion for u in powers of t^ν as $t \to 0$.

A different approach [11, Theorem 2.1], based on a contour integral representation of u and a resolvent estimate for A, yields bounds like (1.8) in the maximum norm; for instance, $t^q \|Au^{(q)}(t)\|_{L_\infty(\Omega)} \le Ct^{-\nu}\|u_0\|_{L_\infty(\Omega)}$, corresponding to the case $\mu = 2$. Cuesta et al. [1] used an essentially similar approach, in the guise of an operational calculus. Beware: $\nu = 1 + \alpha$ in the notation of the former paper [11], whereas $\nu = 1 - \alpha$ in the notation of the latter paper [1].

In Section 5, we suppose that $u_0 = 0$ and allow a nonzero f. Again, we are able to adapt known techniques [8] to the present case, and thereby show that

$$t^q \|u^{(q)}(t)\|_{\dot H^{r+\mu}} \le Ct^{-\mu\nu/2} \sum_{j=0}^{q+1} \int_0^t s^j \|f^{(j)}(s)\|_{\dot H^r}\, ds,$$

for $0 \le \mu \le 2$. The previously cited work [11] proved only a basic estimate for the inhomogeneous problem,

$$\int_0^t \|Au'(s)\|_{L_\infty(\Omega)}\, ds \le Ct^{1-\nu}\Big(\|f(0)\|_{L_\infty(\Omega)} + \int_0^t \|f'(s)\|_{L_\infty(\Omega)}\, ds\Big).$$

Finally, in Section 6 we investigate the behaviour of the solution when the initial datum u_0 does not satisfy the boundary condition, in the simple case when $f \equiv 0$ and the spatial dimension $d = 1$. It follows that $u_0 \in \dot H^r$ only when $r < \frac{1}{2}$ for a Dirichlet boundary condition, and only when $r < \frac{3}{2}$ for a Neumann boundary condition, limiting the applicability of our regularity estimates (1.8).

2. Separation of variables

For much of our analysis, we treat A in (1.5) as an abstract, unbounded, self-adjoint linear operator on a real Hilbert space $\mathbb{H}$. We make the following assumptions:

(1) the eigenfunctions $\phi_0, \phi_1, \phi_2, \ldots$ of A form a complete orthonormal system in $\mathbb{H}$;
(2) the associated eigenvalues $\lambda_0, \lambda_1, \lambda_2, \ldots$ are all nonnegative.

We write $\phi_m = \phi_m^{\mathrm{D}}$ and $\lambda_m = \lambda_m^{\mathrm{D}}$, or $\phi_m = \phi_m^{\mathrm{N}}$ and $\lambda_m = \lambda_m^{\mathrm{N}}$, whenever it is necessary to be specific about the boundary condition, that is,

$$\phi_m^{\mathrm{D}} = 0 \quad \text{and} \quad \frac{\partial \phi_m^{\mathrm{N}}}{\partial n} = 0 \quad \text{on } \partial\Omega.$$

Without loss of generality, we assume for convenience that

$$0 \le \lambda_0 \le \lambda_1 \le \lambda_2 \le \cdots.$$

These assumptions are satisfied in the case $Au = -\nabla \cdot (K\nabla u)$ and $\mathbb{H} = L_2(\Omega)$. Note that $\lambda_0^{\mathrm{D}} > 0$ in the case of the Dirichlet boundary condition (1.3), but $\lambda_0^{\mathrm{N}} = 0$ for the Neumann boundary condition (1.4).

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Denote the inner product and norm in $\mathbb{H}$ by $\langle u, v\rangle$ and $\|u\|$, respectively. It is often convenient to treat u as a function of t taking values in $\mathbb{H}$. Assumption (1) above implies that

$$u(t) = \sum_{m=0}^{\infty} u_m(t)\phi_m \quad \text{where } u_m(t) = \langle u(t), \phi_m\rangle,$$

and we likewise put $f_m(t) = \langle f(t), \phi_m\rangle$ and $u_{0m} = \langle u_0, \phi_m\rangle$.

Taking the inner product of ϕ_m with (1.5) gives a scalar initial-value problem

$$\frac{du_m}{dt} + \lambda_m(\omega_\nu * u_m)_t = f_m(t) \quad \text{for } t > 0, \text{ with } u_m(0) = u_{m0}, \tag{2.1}$$

for each $m \geq 0$. We construct the solution u_m using the Laplace transform,

$$\hat{w}(z) = \mathcal{L}\{w(t)\} = \int_0^\infty e^{-zt} w(t)\, dt.$$

Since $\hat{\omega}_\nu(z) = z^{-\nu}$, problem (2.1) becomes

$$z\hat{u}_m(z) - u_{0m} + \lambda_m z^{1-\nu}\hat{u}_m(z) = \hat{f}_m(z),$$

and so

$$\hat{u}_m(z) = \frac{u_{0m} + \hat{f}_m(z)}{z + \lambda_m z^{1-\nu}}. \tag{2.2}$$

A geometric series expansion shows that, for any constant $\lambda > 0$,

$$\mathcal{L}^{-1}\left\{\frac{1}{z + \lambda z^{1-\nu}}\right\} = E_\nu(-\lambda t^\nu), \tag{2.3}$$

where E_ν is the Mittag-Leffler function [2, pp. 206–212], defined by

$$E_\nu(t) = \sum_{p=0}^{\infty} \frac{t^p}{\Gamma(1 + \nu p)}. \tag{2.4}$$

Therefore, the representation (2.2) implies that

$$u_m(t) = u_{0m}E_\nu(-\lambda_m t^\nu) + \int_0^t E_\nu(-\lambda_m(t-s)^\nu) f_m(s)\, ds, \tag{2.5}$$

leading us to define the linear operator

$$\mathcal{E}(t)w = \sum_{m=0}^{\infty} E_\nu(-\lambda_m t^\nu)\langle w, \phi_m\rangle\phi_m. \tag{2.6}$$

The solution of the fractional diffusion equation (1.5) is then given by the Duhamel formula,

$$u(t) = \mathcal{E}(t)u_0 + \int_0^t \mathcal{E}(t-s)f(s)\, ds. \tag{2.7}$$

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By deforming the integration contour in the Laplace inversion formula, it follows from (2.3) that

$$E_\nu(-t^\nu) = \frac{1}{\pi}\int_0^\infty \frac{e^{-xt}x^{\nu-1}\sin\pi\nu\,dx}{(x^\nu+\cos\pi\nu)^2+\sin^2\pi\nu}; \tag{2.8}$$

see Gorenflo et al. [4, equation (23)]. Hence $E_\nu(-t^\nu)$ is positive and decreasing for $0<t<\infty$, and since $E_\nu(0)=1$ it follows that $0\le E_\nu(-t)\le 1$ for all $t\ge 0$. Thus

$$\|\mathcal{E}(t)w\|^2 = \sum_{m=0}^\infty (E_\nu(-\lambda_m t^\nu)\langle w,\phi_m\rangle)^2 \le \sum_{m=0}^\infty \langle w,\phi_m\rangle^2 = \|w\|^2,$$

and the formal construction above, leading to (2.7), does in fact define a function $u:[0,\infty)\to\mathbb{H}$, satisfying the a priori estimate

$$\|u(t)\| \le \|u_0\| + \int_0^t \|f(s)\|\,ds \quad \text{for } t\ge 0.$$

3. Sobolev spaces

To measure the spatial regularity of $w\in\mathbb{H}$, we introduce the norm $\|w\|_r$ defined by

$$\|w\|_r^2 = \|(I+A)^{r/2}w\|^2 = \sum_{m=0}^\infty (1+\lambda_m)^r\langle w,\phi_m\rangle^2 \quad \text{for } 0\le r<\infty,$$

and define the associated Hilbert space $\dot{H}^r=\{w\in\mathbb{H}:\|w\|_r<\infty\}$.

For the concrete partial differential operator $Au=-\nabla\cdot(K\nabla u)$ and the space $\mathbb{H}=L_2(\Omega)$, we write $\dot{H}^r=\dot{H}^r_{\mathrm{D}}$ if we want to emphasise that $\phi_m=\phi_m^{\mathrm{D}}$, and $\dot{H}^r=\dot{H}^r_{\mathrm{N}}$ if $\phi_m=\phi_m^{\mathrm{N}}$. If Ω is C^∞ then

$$\dot{H}^r_{\mathrm{D}} = H^r(\Omega) \text{ for } 0<r<\tfrac12 \quad \text{and} \quad \dot{H}^r_{\mathrm{N}} = H^r(\Omega) \text{ for } 0<r<\tfrac32, \tag{3.1}$$

and for $j=1,2,3,\ldots,$

$$\dot{H}^r_{\mathrm{D}} = \{w\in H^r(\Omega): w=Aw=\cdots=A^{j-1}w=0 \text{ on } \partial\Omega\} \quad \text{for } 2j-\tfrac32<r<2j+\tfrac12, \tag{3.2}$$

and

$$\dot{H}^r_{\mathrm{N}} = \{w\in H^r(\Omega): \partial_n w=\partial_n Aw=\cdots=\partial_n A^{j-1}w=0 \text{ on } \partial\Omega\} \quad \text{for } 2j-\tfrac12<r<2j+\tfrac32. \tag{3.3}$$

For the exceptional Dirichlet index $r=2j-\frac32$, the condition $A^{j-1}w=0$ on $\partial\Omega$ is replaced by $A^{j-1}w\in\tilde{H}^{1/2}(\Omega)$, and similarly for the exceptional Neumann index $r=2j-\frac12$ the condition $\partial_n A^{j-1}w=0$ on $\partial\Omega$ is replaced by $\partial_n A^{j-1}w\in\tilde{H}^{1/2}(\Omega)$. These results are proved using elliptic regularity theory and interpolation [15, p. 34], [16, Theorem 4.3.3]. If Ω is not C^∞ then we must restrict r accordingly; for instance, if Ω is Lipschitz then the above relations are valid for $r\le 1$, and if Ω is convex or $C^{1,1}$ then we can allow $r\le 2$.

4. Homogeneous problem

In this section, we consider (1.5) when $f(t)\equiv 0$, so that the solution (2.7) reduces to $u(t)=\mathcal{E}(t)u_0$. Our results assume that $u_0\in\dot{H}^r$ for some $r\ge 0$. In practice, for generic, reasonably smooth data, this assumption holds only for $r<\frac12$ in the

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case of a Dirichlet boundary condition, and only for $r < \frac{3}{2}$ in the case of a Neumann boundary condition; see (3.1). If u_0 happens to satisfy the boundary condition, then by (3.2) and (3.3) these restrictions are relaxed to $r < \frac{5}{2}$ and $r < \frac{7}{2}$, respectively.

Let $\lambda_+ = \min\{\lambda_m : \lambda_m > 0\}$ denote the smallest, strictly positive eigenvalue of A. Since $E_\nu(0) = 1$, we make the splitting

$$\mathcal{E}(t) = \mathcal{E}_0 + \mathcal{E}_+(t),$$

where

$$\mathcal{E}_0 w = \sum_{\lambda_m = 0} \langle w, \phi_m \rangle \phi_m \quad \text{and} \quad \mathcal{E}_+(t) w = \sum_{\lambda_m \ge \lambda_+} E_\nu(-\lambda_m t^\nu) \langle w, \phi_m \rangle \phi_m;$$

of course, if $\lambda_0 > 0$, so that $\lambda_+ = \lambda_0$, then $\mathcal{E}_0 = 0$ and $\mathcal{E}_+(t) = \mathcal{E}(t)$. In studying the regularity of $\mathcal{E}(t)w$, it suffices to consider the part $\mathcal{E}_+(t)w$, because

$$\|\mathcal{E}_0 w\|_r = \|\mathcal{E}_0 w\| \le \|w\| \quad \text{for } 0 \le r < \infty.$$

The Mittag-Leffler function admits the asymptotic expansion [2, p. 207]

$$E_\nu(-t) = \sum_{p=1}^{N} \frac{(-1)^{p+1} t^{-p}}{\Gamma(1 - \nu p)} + O(t^{-N-1}) \quad \text{as } t \to \infty, \tag{4.1}$$

so in the sum (2.6) the mth Fourier mode is damped by a factor $E_\nu(-\lambda_m t^\nu) \sim \lambda_m^{-1} t^{-\nu}/\Gamma(1-\nu)$, with the result that for $t > 0$ the solution is smoother than the initial datum, as we see in the next theorem. Here the subscript in C_T emphasises that the constant depends on T; in future we use this notation without further comment.

Theorem 4.1. *Let $0 \le \mu \le 2$ and $0 \le r < \infty$. If $w \in \dot{H}^r$, then*

$$\|\mathcal{E}(t) w\|_{r+\mu} \le C_T t^{-\mu\nu/2} \|w\|_r \quad \textit{for } 0 < t \le T,$$

and

$$\|\mathcal{E}_+(t) w\|_{r+\mu} \le C(1 + \lambda_+^{-1})^{\mu/2} t^{-\mu\nu/2} \|w\|_r \quad \textit{for } 0 < t < \infty.$$

Proof. Put $g(t) = E_\nu(-t^\nu)$, so that

$$\|\mathcal{E}(t) w\|_{r+\mu}^2 = \sum_{m=0}^{\infty} (1 + \lambda_m)^{r+\mu} g(\lambda_m^{1/\nu} t)^2 \langle w, \phi_m \rangle^2.$$

From the series definition (2.4) and the asymptotic expansion (4.1), we see that

$$g(t) \le C \min\{1, t^{-\nu}\} \le C(1 + t^\nu)^{-\mu/2} \quad \text{for } 0 < t < \infty.$$

Thus, if $0 < t \le 1$ then

$$g(\lambda_m^{1/\nu} t)^2 \le C(1 + \lambda_m t^\nu)^{-\mu} = C t^{-\mu\nu} (t^{-\nu} + \lambda_m)^{-\mu} \le C t^{-\mu\nu} (1 + \lambda_m)^{-\mu}$$

and so

$$\|\mathcal{E}(t) w\|_{r+\mu}^2 \le C t^{-\mu\nu} \sum_{m=0}^{\infty} (1 + \lambda_m)^r \langle w, \phi_m \rangle^2 = C t^{-\mu\nu} \|w\|_r^2.$$

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In addition, $g(t) \le Ct^{-\mu\nu/2}$ for $0 < t < \infty$, implying that

$$\begin{aligned} g(\lambda_m^{1/\nu} t)^2 &\le C\lambda_m^{-\mu} t^{-\mu\nu} = Ct^{-\mu\nu}\Big(\frac{1+\lambda_m}{\lambda_m}\Big)^{\mu}(1+\lambda_m)^{-\mu} \\ &\le Ct^{-\mu\nu}(1+\lambda_+^{-1})^{\mu}(1+\lambda_m)^{-\mu} \quad \text{when } \lambda_m > 0, \end{aligned}$$

from which the estimate for $\|\mathcal{E}_+(t)w\|_{r+\mu}$ follows at once. □

In classical diffusion, the mth Fourier mode of the initial datum is damped by a factor $E_1(-\lambda_m t) = e^{-\lambda_m t}$, with the result that $\|u(t)\|_{r+\mu} \le Ct^{-\mu/2}\|u_0\|_r$ for *every* $\mu > 0$. The weaker damping of the high-frequency modes in fractional subdiffusion accounts for the restriction $\mu \le 2$ in Theorem 4.1.

The same method of proof works for the time derivatives of $\mathcal{E}(t)$.

THEOREM 4.2. *Let $-2 \le \mu \le 2$, $0 \le r < \infty$ and $q \in \{1, 2, 3, \ldots\}$. If $w \in \dot H^r$, then*

$$t^q \|\mathcal{E}^{(q)}(t)w\|_{r+\mu} \le C_{q,T} t^{-\mu\nu/2}\|w\|_r \quad \textit{for } 0 < t \le T,$$

and

$$t^q \|\mathcal{E}^{(q)}(t)w\|_{r+\mu} \le C_q(1+\lambda_+^{-1})^{\mu/2} t^{-\mu\nu/2}\|w\|_r \quad \textit{for } 0 < t \le \infty.$$

PROOF. Again, we define $g(t) = E_\nu(-t^\nu)$ so that $g(\lambda^{1/\nu}t) = E_\nu(-\lambda t^\nu)$. For $0 < t < \infty$, the asymptotic expansion (4.1) implies that

$$t^q |g^{(q)}(t)| \le C_q \min\{t^\nu, t^{-\nu}\} \le C_q t^{-\mu\nu/2}.$$

So by the chain rule,

$$\begin{aligned} t^q \Big|\Big(\frac{d}{dt}\Big)^q g(\lambda_m^{1/\nu}t)\Big| &= (\lambda_m^{1/\nu}t)^q |g^{(q)}(\lambda_m^{1/\nu}t)| \le C_q(\lambda_m^{1/\nu}t)^{-\mu\nu/2} = C_q t^{-\mu\nu/2}\lambda_m^{-\mu/2} \\ &\le C_q t^{-\mu\nu/2}(1+\lambda_+^{-1})^{\mu/2}(1+\lambda_m)^{-\mu/2} \quad \text{for } \lambda_m \ge \lambda_+, \end{aligned}$$

and the second estimate follows at once, noting that $\mathcal{E}^{(q)}(t) = \mathcal{E}_+^{(q)}(t)$. To prove the first estimate, we use

$$t^q |g^{(q)}(t)| \le \begin{cases} C_q t^{-\nu\mu/2} & \text{for } -2 \le \mu \le 0 \\ C_q(1+t^\nu)^{-\mu/2} & \text{for } 0 \le \mu \le 2 \end{cases}$$

to obtain

$$\begin{aligned} t^q \Big|\Big(\frac{d}{dt}\Big)^q g(\lambda_m^{1/\nu}t)\Big| &\le \begin{cases} C_q \lambda_m^{-\mu/2} t^{-\mu\nu/2} & \text{for } -2 \le \mu \le 0 \\ C_q(1+\lambda_m t^\nu)^{-\mu/2} & \text{for } 0 \le \mu \le 2 \end{cases} \\ &\le C_q t^{-\mu\nu/2}(1+\lambda_m)^{-\mu/2} \quad \text{for } 0 < t \le 1. \end{aligned}$$

□

The following expansion describes in finer detail the behaviour of $\mathcal{E}(t)v$ as $t \to 0$.

THEOREM 4.3. *Let $0 \le \mu \le 2$ and $0 \le r < \infty$. If $w \in \dot H^{r+2M}$, then*

$$\mathcal{E}(t)w = w + \sum_{p=1}^{M-1} \frac{(-1)^p t^{\nu p}}{\Gamma(1+\nu p)} A^p w + R_M(t)A^M w,$$

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where the operator $R_M(t)$ satisfies

$$\|R_M(t)w\|_{r+\mu} \le C_{M,T} t^{M\nu-\mu\nu/2}\|w\|_r \quad \text{for } 0 < t \le T.$$

PROOF. From (2.4) and (4.1), we see that the function

$$g_M(t) = t^{-M\nu}\biggl(E_\nu(-t^\nu) - \sum_{p=0}^{M-1} \frac{(-1)^p t^{\nu p}}{\Gamma(1+\nu p)}\biggr)$$

satisfies $|g_M(t)| \le C_M \min\{1, t^{-\nu}\}$. Since

$$E_\nu(-\lambda t^\nu) = 1 + \sum_{p=1}^{M-1} \frac{(-1)^p t^{\nu p}}{\Gamma(1+\nu p)}\, \lambda^p + t^{M\nu} g_M(\lambda^{1/\nu} t)\lambda^M,$$

we may estimate $\|R_M(t)w\|_{r+\mu}$ by the same method as in the proof of Theorem 4.1. □

Notice that the case $M = 1$ with $r = 0$ and $\mu = 2 - \alpha$ gives the estimate

$$\|w - \mathcal{E}(t)w\|_{2-\alpha} \le Ct^{\nu-(2-\alpha)\nu/2}\|Aw\| = Ct^{\alpha\nu/2}\|Aw\| \quad \text{for } 0 \le \alpha \le 2,$$

and since $\mathcal{E}(t)$ commutes with $(I + A)^{(\alpha-2)/2}$,

$$\|w - \mathcal{E}(t)w\| \le Ct^{\alpha\nu/2}\|w\|_\alpha \quad \text{for } 0 \le \alpha \le 2,$$

showing that $\mathcal{E}(t)w \to w$ in $\mathbb{H}$ if $w \in \dot{H}^r$ for any $r > 0$.

To conclude this section, we show that bounds of the form (1.6) and (1.7) hold.

THEOREM 4.4. *If $\sigma = r\nu/2$ and $q \in \{1, 2, 3, \dots\}$, then for $0 < t \le T$ the solution of the homogeneous problem, $u(t) = \mathcal{E}(t)u_0$, satisfies*

$$t^{q-1+\nu}\|Au^{(q)}(t)\| \le C_{q,T} t^{\sigma-1}\|u_0\|_r \quad \text{for } 0 \le r \le 4,$$

and

$$t^{q-1}\|u^{(q)}(t)\| \le C_{q,T} t^{\sigma-1}\|u_0\|_r \quad \text{for } 0 \le r \le 2.$$

PROOF. The first estimate follows by taking $\mu = 2 - r$ in Theorem 4.2, and the second by taking $\mu = -r$. □

5. Inhomogeneous problem

We now consider (1.5) with $u_0 = 0$ and nonzero f, so that (2.7) reduces to

$$u(t) = \int_0^t \mathcal{E}(t-s) f(s)\, ds. \tag{5.1}$$

For our regularity estimates, we make use of several lemmas involving the differential operator D defined by

$$Dw(t) = tw'(t).$$

The first shows that the bounds of Theorem 4.2 hold with $t^q\mathcal{E}^{(q)}(t)$ replaced by $D^q\mathcal{E}(t)$.

LEMMA 5.1. *For $q \in \{1, 2, 3, \dots\}$ there exist constants a_{qj} and b_{qj} such that*

$$D^q w(t) = \sum_{j=1}^{q} a_{qj} t^j w^{(j)}(t) \quad \text{and} \quad t^q w^{(q)}(t) = \sum_{j=1}^{q} b_{qj} D^j w(t).$$

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PROOF. Use induction on q. ◻

The next lemma shows how D acts on a convolution.

LEMMA 5.2. *We have the following identities:*

(1) $D(v * w) = v * w + (Dv) * w + v * (Dw)$;
(2) $D\omega_\mu = (\mu - 1)\omega_\mu$;
(3) $D(\omega_\mu * v) = \omega_\mu * (D + \mu)v$.

PROOF. We observe that

$$\frac{\partial}{\partial t}\int_0^t v(t-s)w(s)\,ds = v(0)w(t) + \int_0^t v'(t-s)w(s)\,ds,$$

so

$$D(v * w)(t) = v(0)tw(t) + \int_0^t (Dv)(t-s)w(s)\,ds + \int_0^t sv'(t-s)w(s)\,ds.$$

Integration by parts gives

$$\int_0^t sv'(t-s)w(s)\,ds = -v(0)tw(t) + (v * w)(t) + (v * Dw)(t),$$

implying the identity in part (1). For part (2) we have

$$D\omega_\mu(t) = t\omega_\mu'(t) = t(\mu-1)t^{\mu-2}/\Gamma(\mu) = (\mu-1)\omega_\mu(t),$$

and together these first two results give

$$D(\omega_\mu * v) = \omega_\mu * v + (\mu - 1)\omega_\mu * v + \omega_\mu * (Dv) = \omega_\mu * (\mu v + Dv),$$

proving part (3). ◻

Applying D^q to a convolution yields a sum of the following form.

LEMMA 5.3. *There exist constants a_{qjk} such that*

$$D^q(v * w) = \sum_{j+k\le q} a_{qjk}(D^j v) * (D^k w).$$

PROOF. We again use induction on q. Part (1) of Lemma 5.2 shows that the case $q = 1$ holds with $a_{100} = a_{110} = a_{101} = 1$, and that

$$D[(D^j v) * (D^k w)] = (D^j v) * (D^k w) + (D^{j+1} v) * (D^k w) + (D^j v) * (D^{k+1} w),$$

from which the inductive step follows at once. ◻

We now prove the analogue of Theorems 4.1 and 4.2 with $\mu = 0$.

THEOREM 5.4. *Let $0 \le r < \infty$ and $q \in \{0, 1, 2, \ldots\}$. Then*

$$t^q\|(\mathcal{E} * f)^{(q)}(t)\|_r \le C_q \sum_{j=0}^{q} \int_0^t s^j\|f^{(j)}(s)\|_r\,ds \quad \textit{for } 0 < t < \infty.$$

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Proof. Taking $\mu = 0$ in Theorems 4.1 and 4.2, we have $\|D^q\mathcal{E}(t)w\|_r \le C_q\|w\|_r$. So by Lemma 5.3,

$$\|D^q(\mathcal{E} * f)\|_r \le C_q \sum_{j+k\le q} \int_0^t \|(D^jE)(t-s)(D^kf)(s)\|_r\,ds \le C_q \sum_{j=0}^{q} \int_0^t \|D^jf(s)\|_r\,ds,$$

and the result follows by Lemma 5.1. □

The preceding proof easily generalizes to show that

$$t^q\|(\mathcal{E} * f)^{(q)}(t)\|_{r+\mu} \le C_q \sum_{j=0}^{q} \int_0^t (t-s)^{-\mu\nu/2} s^j \|f^{(j)}(s)\|_r\,ds$$

for $0 \le \mu \le 2$ if $q = 0$, and for $-2 \le \mu \le 2$ if $q \ge 1$. However, we derive an alternative bound in which the factor $(t-s)^{-\mu\nu/2}$ in the integrand is replaced by $t^{-\mu\nu/2}$ (for $0 \le \mu \le 2$), at the cost of adding a term with $j = q + 1$.

We integrate (1.5) with respect to t, remembering that $u_0 = 0$, to see that $u = \mathcal{E} * f$ satisfies

$$u + \omega_\nu * Au = F \quad \text{where } F(t) = \int_0^t f(s)\,ds.$$

Since $\omega_{1-\nu} * \omega_\nu = \omega_1$, it follows that

$$\omega_1 * Au = \omega_{1-\nu} * \omega_\nu * Au = \omega_{1-\nu} * (F - u),$$

or in other words,

$$\int_0^t Au(s)\,ds = \int_0^t \frac{(t-s)^{-\nu}}{\Gamma(1-\nu)}[F(s) - u(s)]\,ds.$$

Using part (3) of Lemma 5.2,

$$D(\omega_1 * Au) = D(\omega_{1-\nu} * (F - u)) = \omega_{1-\nu} * (D + 1 - \nu)(F - u),$$

implying that

$$tAu(t) = \int_0^t \frac{(t-s)^{-\nu}}{\Gamma(1-\nu)}(D + 1 - \nu)[F(s) - u(s)]\,ds. \tag{5.2}$$

The desired estimate is obtained by using this representation and the following identities.

Lemma 5.5. *There exist constants c_{qj} such that*

$$t^q w^{(q)}(t) = t^{-1} \sum_{j=0}^{q} c_{qj} D^j(tw) \quad \textit{and} \quad D^q(tw) = t \sum_{j=0}^{q} \binom{q}{j} D^j w.$$

Proof. Use induction on q. □

We now arrive at the main result for this section.

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Theorem 5.6. *Let* $0 \le \mu \le 2$, $0 \le r < \infty$ *and* $q \in \{0, 1, 2, \ldots\}$. *Then*

$$t^q \|(\mathcal{E} * f)^{(q)}(t)\|_{r+\mu} \le C_{q,\nu}(1 + t^{-\mu\nu/2}) \sum_{j=0}^{q+1} \int_0^t s^j \|f^{(j)}(s)\|_r \, ds.$$

Proof. Put $u = \mathcal{E} * f$. The first identity in Lemma 5.5 shows that to bound $t^q\|u^{(q)}(t)\|_{r+2}$ it suffices to consider

$$t^{-1}\|D^q(tu)\|_{r+2} = t^{-1}\|(I + A)D^q(tu)\|_r \le t^{-1}\|D^q(tu)\|_r + t^{-1}\|D^q(tAu)\|_r.$$

The second identity in Lemma 5.5 and the fact that, by (5.2),

$$D^q(tAu) = D^q(\omega_{1-\nu} * (D + 1 - \nu)(F - u)) = \omega_{1-\nu} * (D + 1 - \nu)^{q+1}(F - u)$$

then give

$$t^{-1}\|D^q(tu)\|_{r+2} \le C_q\Big(\sum_{j=0}^{q} \|D^j u\|_r + t^{-1} \sum_{j=0}^{q+1} \omega_{1-\nu} * \|D^j(F - u)\|_r\Big),$$

in which the first sum may be estimated using Theorem 5.4.

Part (2) of Lemma 5.2 and Lemma 5.3 give

$$D^j(F - u) = D^j(\omega_1 * f - \mathcal{E} * f) = \omega_1 * (D + 1)^j f - \sum_{k+l\le j} a_{jkl}(D^k\mathcal{E}) * (D^l f).$$

Therefore, by Theorem 4.1,

$$\|D^j(F - u)\|_r \le C_j \sum_{k=0}^{j} \int_0^t \|D^k f(s)\|_r \, ds = C_j \sum_{k=0}^{j} \omega_1 * \|D^k f\|_r$$

and hence

$$t^{-1}\omega_{1-\nu} * \|D^j(F - u)\|_r \le C_j \sum_{k=0}^{j} t^{-1}\omega_{2-\nu} * \|D^k f\|_r.$$

Since $\omega_{2-\nu} * \|D^k f\|_r \le C t^{1-\nu} \int_0^t \|D^k f(s)\|_r \, ds$, we conclude that

$$t^{-1}\|D^q(tu)\|_{r+2} \le C_q(1 + t^{-\nu}) \sum_{j=0}^{q+1} \int_0^t \|D^j f(s)\|_r \, ds$$

and thus

$$t^q\|u^{(q)}(t)\|_{r+2} \le C_q \sum_{j=0}^{q} t^{-1}\|D^j(tu)\|_{r+2} \le C_q(1 + t^{-\nu}) \sum_{j=0}^{q+1} \int_0^t \|D^j f(s)\| \, ds,$$

proving the result in the case $\mu = 2$. The general case follows by Theorem 5.4 using the interpolation inequality

$$\|w\|_{r+\mu} \le (\|w\|_r)^{1-\mu/2}(\|w\|_{r+2})^{\mu/2}. \qquad \square$$

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We further investigate the behaviour of $\mathcal{E} * f$ as $t \to 0$ using the expansion of $\mathcal{E}(t)w$ given in Theorem 4.3. For instance, if

$$f(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)} w = \omega_\alpha(t) w \quad \text{for } \alpha > 0 \text{ and } w \in \dot{H}^{r+2M},$$

then

$$\begin{aligned} \mathcal{E} * f &= \Big(\sum_{p=0}^{M-1} (-1)^p \omega_{1+\nu p} A^p + R_M A^M \Big) * \omega_\alpha w \\ &= \sum_{p=0}^{M-1} (-1)^p \omega_{1+\nu p+\alpha} A^p w + R_M * \omega_\alpha A^M w; \end{aligned}$$

that is, since $\|R_M * \omega_\alpha A^M w\|_r \le C\omega_{1+\nu M} * \omega_\alpha \|A^M w\|_r \le C\omega_{1+\nu M+\alpha}\|w\|_{r+2M}$,

$$(\mathcal{E} * f)(t) = \frac{t^\alpha}{\Gamma(1+\alpha)} w + \sum_{p=1}^{M-1} \frac{(-1)^p t^{\nu p+\alpha}}{\Gamma(1+\nu p+\alpha)} A^p w + O(t^{\nu M+\alpha}) \quad \text{as } t \to 0.$$

As for the homogeneous problem, we have bounds of the form (1.6) and (1.7).

Theorem 5.7. *If $\sigma = r\nu/2$, $0 \le r \le 2$ and $q \in \{1, 2, 3, \ldots\}$, then the solution $u = \mathcal{E} * f$ of the inhomogeneous problem with $u_0 = 0$ satisfies*

$$t^{q-1+\nu} \|Au^{(q)}(t)\| \le C_{q,T} t^{\sigma-1} \sum_{j=0}^{q+1} \int_0^t s^j \|f^{(j)}(s)\|_r \, ds$$

and

$$t^{q-1} \|u^{(q)}(t)\| \le C_{q,T} t^{\sigma-1} \sum_{j=0}^{q} \int_0^t s^{j-\sigma} \|f^{(j)}(s)\| \, ds$$

for $0 < t \le T$.

Proof. Take $\mu = 2 - r$ in Theorem 5.6 for the first estimate, and use Theorem 5.4 with $r = 0$ for the second, noting that

$$\int_0^t s^j \|f^{(j)}(s)\| \, ds \le t^\sigma \int_0^t s^{j-\sigma} \|f^{(j)}(s)\| \, ds. \qquad \square$$

The preceding analysis assumes that $f(t)$ is sufficiently smooth as a function of t for $t > 0$. For an example of what happens if this assumption is not satisfied, suppose that f is piecewise smooth with just a single jump discontinuity at $t = a$ for some $a > 0$. Writing $[f]_a = f(a^+) - f(a^-)$,

$$Df(t) = a[f]_a \delta(t-a) + w(t)$$

where w is piecewise smooth, and so by Lemma 5.2,

$$D(\mathcal{E} * f)(t) = a\mathcal{E}(t-a)[f]_a + (\mathcal{E} * f + (D\mathcal{E}) * f + \mathcal{E} * w)(t) \quad \text{for } t > a.$$

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6. Incompatible initial data

We describe the behaviour of the solution when the initial datum u_0 is not compatible with the given boundary condition, in the simple case when the spatial domain is the positive half-axis $\Omega = (0, \infty)$, and $f(t) \equiv 0$.

Consider first the case $\Omega = (-\infty, \infty)$, that is,

$$u_t - K(\omega_\nu * u_{xx})_t = 0 \quad \text{and} \quad u(x, 0) = u_0(x),$$

for $-\infty < x < \infty$ and $t > 0$, with $u(x, t)$ bounded as $x \to \pm\infty$. Denoting the Fourier transform of u by

$$\tilde{u}(\xi, t) = \mathcal{F}\{u(x, t)\} = \int_{-\infty}^{\infty} e^{-i\xi x} u(x, t)\, dx,$$

we see that

$$\tilde{u}_t + K\xi^2(\omega_\nu * \tilde{u})_t = 0 \quad \text{with } \tilde{u}(\xi, 0) = \tilde{u}_0(\xi).$$

Thus, $\tilde{u}$ satisfies an equation having the same form as (2.1), except that $K\xi^2$ takes the place of λ_m, and no source term is present. Hence, by (2.5),

$$\tilde{u}(\xi, t) = E_\nu(-K\xi^2 t^\nu)\tilde{u}_0(\xi),$$

and therefore

$$u(x, t) = \int_{-\infty}^{\infty} G(x - y, t) u_0(y)\, dy, \tag{6.1}$$

where the Green function, or fundamental solution, is given by

$$G(x, t) = \mathcal{F}^{-1}\{E_\nu(-K\xi^2 t^\nu)\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi x} E_\nu(-K\xi^2 t^\nu)\, d\xi. \tag{6.2}$$

The inverse Fourier transform (6.2) may be expressed in terms of the M-Wright function [7],

$$M_\alpha(x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n!\Gamma(1 - \alpha(n + 1))} = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n-1} x^{n-1}}{(n - 1)!} \Gamma(\alpha n) \sin(\pi\alpha n),$$

where the identity $\Gamma(z)\Gamma(1 - z) = \pi/\sin(\pi z)$ shows that the two series are equal. In fact [7, Section 4.5],

$$\mathcal{F}\{M_\alpha(|x|)\} = 2E_{2\alpha}(-\xi^2) \quad \text{for } 0 < \alpha < 1,$$

so

$$G(x, t) = \frac{1}{2\sqrt{Kt^\nu}} M_{\nu/2}\Big(\frac{|x|}{\sqrt{Kt^\nu}}\Big).$$

Notice that for each $t > 0$, the function $x \mapsto G(x, t)$ is not differentiable at $x = 0$. However, in the limiting case when $\nu \to 1$, we have $M_{1/2}(x) = \pi^{-1/2} \exp(-x^2/4)$ and $G(x, t)$ is just the classical heat kernel, which is C^∞ for $t > 0$.

The behaviour of $G(x, t)$ for large x may be seen from the asymptotic formula [7, equation (4.5)]

$$M_\alpha(x/\alpha) \sim \frac{x^{(\alpha-1/2)/(1-\alpha)}}{\sqrt{2\pi(1 - \alpha)}} \exp\Big(-\frac{(1 - \alpha)r^{1/(1-\alpha)}}{\alpha}\Big) \quad \text{as } x \to \infty,$$

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where $0 < \alpha < 1$. It follows that the integral (6.1) converges for $t > 0$ if u_0 is locally integrable and bounded on $(-\infty, \infty)$.

Now consider the problem on the half-line $\Omega = (0, \infty)$ with a Dirichlet boundary condition,

$$u_t - K(\omega_\nu * u_{xx})_t = 0, \quad u(x, 0) = u_0(x), \quad u(0, t) = 0, \tag{6.3}$$

for $0 < x < \infty$ and $t > 0$. By taking the odd extension of the initial datum to $(-\infty, \infty)$, so that $u_0(-x) = -u_0(x)$, we obtain the solution to (6.3),

$$u(x, t) = \int_{-\infty}^{\infty} G(x - y, t) u_0(y)\, dy = \int_0^{\infty} [G(x - y, t) - G(x + y, t)] u_0(y)\, dy.$$

Suppose now that $u_0(0) \neq 0$. This means that u_0 fails to satisfy the boundary condition, and so $u(x, t)$ is discontinuous at $(x, t) = (0, 0)$. To see the nature of the discontinuity, we rewrite the solution as

$$u(x, t) = \int_{-\infty}^{x} G(y, t) u_0(x - y)\, dy - \int_x^{\infty} G(y, t) u_0(y - x)\, dy.$$

Let $\psi(x, t)$ denote the solution in the special case when $u_0(x) = 1$ for all $x > 0$, that is,

$$\psi(x, t) = \int_{-\infty}^{x} G(y, t)\, dy - \int_x^{\infty} G(y, t)\, dy. \tag{6.4}$$

In the general case,

$$u(x, t) = u_0(0)\psi(x, t) + w(x, t),$$

where w is the solution with initial datum $u_0(x) - u_0(0)$, and is therefore continuous at $(0, 0)$. Since

$$\int_{-\infty}^{\infty} G(y, t)\, dy = \tilde{G}(0, t) = E_\nu(0) = 1,$$

we can simplify (6.4),

$$\psi(x, t) = 1 - 2\int_x^{\infty} G(y, t)\, dy = 1 - \frac{1}{\sqrt{Kt^\nu}} \int_x^{\infty} M_{\nu/2}\Big(\frac{|y|}{\sqrt{Kt^\nu}}\Big)\, dy,$$

and obtain ψ in the form of a similarity solution,

$$\psi(x, t) = \Psi\Big(\frac{x}{\sqrt{Kt^\nu}}\Big) \quad \text{where } \Psi(x) = 1 - \int_x^{\infty} M_{\nu/2}(y)\, dy.$$

If we fix $t > 0$ and let $x \to 0$, then $\psi(x, t) \to \Psi(0) = 0$, whereas if we fix $x > 0$ and let $t \to 0$, then $\psi(x, t) \to \Psi(\infty) = 1$.

To handle a Neumann boundary condition, $u_x(0, t) = 0$, we proceed in the same way except that we use the *even* extension of u_0, so that $u_0(-x) = u_0(x)$ and

$$\begin{aligned} u(x, t) &= \int_0^{\infty} [G(x - y, t) + G(x + y, t)] u_0(y)\, dy \\ &= \int_{-\infty}^{x} G(y, t) u_0(x - y)\, dy + \int_x^{\infty} G(y, t) u_0(y - x)\, dy. \end{aligned}$$

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Although $u(x, t) \to u(0, 0) = u_0$ as $(x, t) \to (0, 0)$, the derivative

$$u_x(x, t) = \int_{-\infty}^{x} G(y, t)u_0'(x - y)\, dy - \int_{x}^{\infty} G(y, t)u_0'(y - x)\, dy$$

is discontinuous at $(0, 0)$. In the special case $u_0(x) = x$ for $x > 0$, we have $u_x(x, t) = \psi(x, t)$, and in general

$$u_x(x, t) = u_{0x}(0)\psi(x, t) + w(x, t),$$

with w continuous at $(0, 0)$.

7. Conclusion

We have seen that solutions of a fractional diffusion equation are less regular than those of its classical counterpart. Underlying our various technical estimates are, first, the representation (2.5) of the mth mode of the solution and, second, the behaviour of the Mittag-Leffler function, shown by the power series (2.4) and the asymptotic expansion (4.1). The high-frequency modes are less strongly damped than in classicial diffusion, reducing the spatial regularity of the solution, and in addition the time derivatives of the solution are generally unbounded as $t \to 0$. Effective numerical methods must take account of this behaviour.

Acknowledgements

The author thanks the Max-Planck-Institut für Mathematik in den Naturwissenchaften, Leipzig, for their hospitality and support during the preparation of this paper.

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